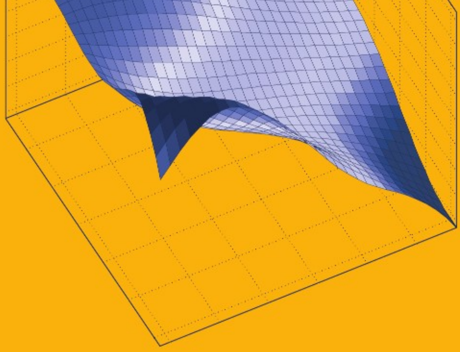
Lecture Notes in Mathematics

J. W. Neuberger

Sobolev Gradients and Differential Equations

1670

2nd Edition



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Preface

What is expected from a theory of differential equations? Look first at the fundamental theorem for ordinary differential equations:

Theorem 0.1. *Suppose that n is a positive integer and G is an open subset of $R \times R^n$ which contains a point (c, w). Suppose also that $f : G \to R^n$ is a continuous function for which there is $M > 0$ such that*

$$\|f(t,x) - f(t,y)\| \leq M\|x - y\| \text{ for all } (t,x),(t,y) \in G. \tag{0.1}$$

Then there is an open interval (a, b) containing c for which there is a unique function u on (a, b) so that

$$u(c) = w, \ u'(t) = f(t, u(t)), \ t \in (a, b).$$

This result can be proved in several constructive ways which yield, along the way, error estimates giving a basis for numerical computation of solutions. Now this existence and uniqueness result certainly does not solve all problems in ordinary differential equations. For one thing, the result is only local. For just one other instance, it doesn't tell about two point boundary value problems, even though it has relevance there. Nevertheless, it provides a position of strength from which to study a wide variety of ordinary differential equations. The fact of existence and uniqueness of a solution gives us something to study in a qualitative, numerical or algebraic setting. The constructive nature of arguments for the above result gives one a good start toward discerning properties of solutions.

Many agree that it would be good to have a similar position of strength for partial differential equations but such does not now exist. It has been argued that there cannot be a central theory of partial differential equations since there is such a great variety of problems. To such an argument I reply that the same opinion about ordinary differential equations was probably held not so much more than a century ago.

These notes are devoted to a description of Sobolev gradients for a variety of problems in differential equations. Sobolev gradients are used in descent processes to find zeros or critical points of functions which in turn provide solutions to underlying differential equations. Our gradients are generally given constructively and do not require full boundary conditions (*i.e.*, conditions which are necessary and sufficient for existence and uniqueness) to be known beforehand. The processes tend to converge in some (non-Euclidean) sense to a nearest solution. The methods apply in cases which are mixed hyperbolic and elliptic — even cases in which regions of hyperbolicity and ellipticity are determined by nonlinearities. Applications to the problem of transonic flow will illustrate this. Numerics are a natural part of the development given here. In fact, numerics are in a sense ahead of theory, giving a spur to more inquiry.

So, do we arrive at a position of strength for fairly general partial differential equations? Here at least is a shadow of such a theory.

A key thing for a reader to keep in mind is that continuous steepest descent with Sobolev gradients is expressed as an ordinary differential equations in a function space whereas alternative descent methods are often partial differential equations themselves (for example, see Chapter 16 in the case of minimal surface problems).

Notes for Second Edition

The theory of Sobolev gradients has developed a great deal since the publication of the first edition of these notes. Many of these developments are reflected in this second edition, which is about twice the length of the first one.

- The use of Sobolev gradients to find critical points of the Ginzburg-Landau energy functional of superconductivity has greatly expanded. It is now near the design stage for superconducting devices. P. Kazemi's recent discoveries play a substantial role here.
- The treatment of Newton's method in the context of Sobolev gradients has been expanded to include a version of the Nash-Moser inverse function theorem. The problem of 'loss of derivatives' has been avoided entirely, a fact that leads to a relatively simple argument for such inverse function results when applied to differential equations. It was first pointed out by A. Castro that considerations for gradient inequalities have much in common with Moser's development of an inverse function theorem.
- The Tricomi equation, showing both elliptic and hyperbolic regions, has been treated using Sobolev gradients.
- A number of new convergence results for continuous steepest descent are included.
- Work on the hyperbolic Monge-Ampere equation, due to T. Howard, is described. This work opens up a new aspect of the study of such equations.
- Use of Sobolev gradients for nonlinear Schrödinger equations is noted.
- A greatly expanded list of properties of the imbedding operator which connects a Hilbert space with a dense linear subspace which is a Hilbert space in its own right. Much of this is due to P. Kazemi.

- After the first edition of this work was published, it was realized that this author's previous use of what is called 'gradient inequality' was preceded by Łojasiewicz inequalities in finite dimensions.
- There is reference to gradient inequality results work of S. Huang and of R. Chill.
- There is an account of Chan-Hilliard equations by S. Sial, T. Lookman, A. Saxena and the present writer.
- There are Sobolev gradient results for fractal regions.
- Some least squares results are given which have application to the problem of separating actual chaos from apparent chaos induced by discretization.
- A new result is given which relates nonlinear semigroup theory to the problem of boundary or supplementary conditions for partial differential equations.

In the first edition, several authors contributed sections on their work with Sobolev gradients. In the second edition, several have kindly agreed to write a chapter on their work. These include

- A development of numerical integration by means of Sobolev gradients, by Ian Knowles and Robert Wallace.
- A discussion of relationships between Sobolev gradients and preconditioning, by Janos Karatson.
- A presentation of curve fitting in the context of Sobolev gradients, by Robert Renka.
- Results on sign changing solutions and Morse index problems, by John M. Neuberger.
- Oil-water separation, elasticity and Model A problems, by Sultan Sial.

Robert Renka and I have had regular discussions about Sobolev gradients for more than two decades. Many others, particularly John M. Neuberger, have read portions of these notes and have contributed corrections and helpful suggestions. Any remaining errors and obscurities are mine. Many students, colleagues, collaborators and others have provided substantial insights. Any attempt at a list acknowledging this help would contain many names but would likely be inadequate. Hence I have decided to not try to make such a list.

I express profound gratitude to Springer for their help and extraordinary patience.

Contents

Chapter 1
Several Gradients

These notes contain an introduction to the idea of Sobolev gradients and how they can be used in the study of differential equations. Numerical considerations are at once a motivation, an investigative tool and an application for this work.

First recall some facts about ordinary gradients. Suppose that for some positive integer n, ϕ is a real-valued $C^{(1)}$ function on R^n. It is customary to define the gradient $\nabla\phi$ as the function on R^n so that if $x = (x_1, x_2, ..., x_n)$ is in R^n, then

$$(\nabla\phi)(x) = \begin{pmatrix} \phi_1(x_1, \cdots, x_n) \\ \vdots \\ \phi_n(x_1, \cdots, x_n) \end{pmatrix} \tag{1.1}$$

where $\phi_i(x_1, ..., x_n)$ is written in place of $\partial\phi/\partial x_i$, $i = 1, 2, ..., n$.

The gradient $\nabla\phi$ has the property that

$$\lim_{t\to 0} \frac{1}{t}(\phi(x + th) - \phi(x)) = \phi'(x)h = \langle h, (\nabla\phi)(x)\rangle_{R^n},\ x, h \in R^n, \tag{1.2}$$

and

$$\|(\nabla\phi)(x)\|_{R^n} = \sup_{h\in R^n, \|h\|_{R^n}=1} |\phi'(x)h|,\ x, h \in R^n.$$

Note that (1.2) can be taken as an equivalent definition of $\nabla\phi$.

For ϕ as above but with $\langle\cdot,\cdot\rangle_S$ an inner product on R^n different from the standard inner product $\langle\cdot,\cdot\rangle_{R^n}$, there is a function $\nabla_S\phi : R^n \to R^n$ so that

$$\phi'(x)h = \langle h, (\nabla_S\phi)(x)\rangle_S,\ x, h \in R^n$$

since the linear functional $\phi'(x)$ can be represented using any inner product on R^n. Say that $\nabla_S\phi$ is the gradient of ϕ with respect to the inner product $\langle\cdot,\cdot\rangle_S$ and note that the gradient $\nabla_S\phi$ has properties similar to those of the ordinary gradient $\nabla\phi$ above except for expression, (1.1).

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_1,

From linear algebra, there is a linear transformation

$$A : R^n \to R^n$$

which relates these two inner products in such a way that if $x, y \in R^n$, then

$$\langle x, y\rangle_S = \langle x, Ay\rangle_{R^n}.$$

Some reflection leads to

$$(\nabla_S \phi)(x) = A^{-1}(\nabla\phi)(x),\ x \in R^n. \tag{1.3}$$

Taking a cue from Riemannian geometry, one can have for each $x \in R^n$ an inner product

$$\langle \cdot, \cdot\rangle_x$$

on R^n. That is, each point of R^n can have its own inner product space. Consider such an assignment made together with a selection of a real-valued C^1 function ϕ on R^n. Then for $x \in R^n$, define $\nabla_x \phi : R^n \to R^n$ so that

$$\phi'(x)h = \langle h, (\nabla_x \phi)(x)\rangle_x,\ x, h \in R^n.$$

For such a gradient system to be of much interest, the corresponding family of inner products, one inner product for each member of R^n, should be related to each other in an orderly way. This is similar to the case of Riemannian geometry in which it is required that inner products be assigned to tangent spaces in a differentiable fashion. In later chapters there are some natural assignments of inner product spaces, some related to Newton's method, and some related to minimal surface problems.

Concrete aspects of the above discussion begin in the following chapter and continue throughout these notes. Most of these considerations apply to Hilbert spaces and, in a somewhat limited way, to more general spaces. Finite dimensional cases are for us synonymous with numerical considerations.

A central theme in these notes is that a given function ϕ has a variety of gradients depending on choice of metric. More to the point, these various gradients have vastly different numerical and analytical properties even when arising from the same function. I first encountered the idea of variable metric in [174] where, in a descent process, different metrics are chosen as a process develops. Karmarkar [96] has used the idea with great success in a linear programming algorithm. In [104] and others, Karmarkar's ideas are developed further. This writer has developed this idea (with differential equations in mind) in a series of papers starting in [145] (or maybe in [141]) and leading to [159, 161, 163]. Variable metrics are related to the conjugate gradient method [80]. Some other classical references to steepest descent are [38, 50, 208].

A 'Sobolev gradient of ϕ' is a gradient of a ϕ when its domain is a finite or infinite dimensional Sobolev space.

There are two related versions of steepest descent. The earliest reference known to me for steepest descent is Cauchy [38]. The first version is discrete steepest descent, the second is continuous steepest descent.

Suppose one has an inner product $\langle \cdot, \cdot \rangle_S$ on a Hilbert space H, a real-valued C^1 function ϕ on H and its gradient $\nabla_S \phi$. By 'discrete steepest descent' is meant an iterative process

$$x_n = x_{n-1} - \delta_{n-1}(\nabla_S \phi)(x_{n-1}),\ n = 1, 2, 3, ..., \tag{1.4}$$

where x_0 is given and δ_{n-1} is chosen to be the number δ which minimizes, if possible,

$$\phi(x_{n-1} - \delta(\nabla_S \phi)(x_{n-1})),\ \delta \in R.$$

On the other hand, continuous steepest descent consists of finding a function $z : [0, \infty) \to H$ so that

$$z(0) = x \in H, z'(t) = -(\nabla_S \phi)(z(t)),\ t \geq 0. \tag{1.5}$$

Continuous steepest descent may be interpreted as a limiting case of (1.4) in which, roughly speaking, various δ_n tend to zero (rather than being chosen optimally). Conversely, (1.4) might be considered (without the optimality condition on δ) as a numerical method (Euler's method) for approximating solutions to (1.5).

Using (1.4) one seeks $u = \lim_{n\to\infty} x_n$ so that

$$\phi(u) = 0 \tag{1.6}$$

or

$$(\nabla_S \phi)(u) = 0. \tag{1.7}$$

Using (1.5) one seeks $u = \lim_{t\to\infty} z(t)$ so that (1.6) or (1.7) holds. Before more general forms of gradients are considered (for example where A in (1.3) is nonlinear), Chapter 2 gives an example intended to convince a reader that there are substantial issues concerning Sobolev gradients. It is hoped that Chapter 2 provides motivation for further reading even though later developments do not depend on proofs in Chapter 2. These arguments might be skipped in a first reading.

This introduction is closed with the indication of two applications of steepest descent:

(a) Many systems of differential equations have a variational principle, *i.e.* there is a function ϕ such that u satisfies the system if and only if u is a critical point of ϕ. In such cases one tries to use steepest descent to find a zero of a gradient of ϕ.

(b) In other problems a system of nonlinear differential equations is written in the form

$$F(x) = 0, \tag{1.8}$$

where F maps a Banach space H of functions into another such space K. In some cases one might define for some $p > 1$, a function $\phi : H \to R$ by

$$\phi(x) = \frac{1}{p}\|F(x)\|_H^p, \; x \in H.$$

and then seek x satisfying (1.8) by means of steepest descent.

Problems of both kinds are considered. The following chapter contains an example of the second kind.

Chapter 2
Comparison of Two Gradients

This chapter gives a comparison between conventional and Sobolev gradients for a finite dimensional problem associated with a simple differential equation. On first reading one might examine just enough to understand the statements of the two theorems. Nothing in the following chapters depends on the techniques of the proofs of these results. Although I expect similar theorems to exist for most systems of differential equations.

In this chapter, all norms and inner products which do not have a subscript are standard Euclidean.

Suppose that ϕ is a $C^{(2)}$ real-valued function on R^n and $\nabla_S\phi$ is the gradient associated with ϕ by means of the positive definite symmetric matrix A, as in the previous chapter. A measure of worth of $\nabla_S\phi$ in regard to a descent process is

$$\sup_{x\in R^n,\phi(x)\neq 0} \frac{\phi(x-\delta_x(\nabla_S\phi)(x))}{\phi(x)} \tag{2.1}$$

where, for each $x \in R^n$, $\delta_x \in R$ is chosen optimally, i.e. a number δ which minimizes

$$\phi(x-\delta(\nabla_S\phi)(x)),\ \delta > 0 \tag{2.2}$$

or, perhaps, is the least positive critical point of the above indicated function. Generally, the smaller the value in (2.1), the greater the worst case improvement in each discrete steepest descent step. It is remarked that $(\nabla_S\phi)(x)$ is a descent direction at x (unless $(\nabla_S\phi)(x) = 0$) since if

$$f(\delta) = \phi(x-\delta(\nabla_S\phi)(x)), \delta \geq 0,$$

then

$$f'(0) = -\|(\nabla_S\phi)(x)\|_S^2 < 0.$$

Equation (2.1) is used to compare performance of two gradients arising from the same function ϕ. For a simple example, choose ϕ so that

$$\phi(u) = u' - u \text{ on } [0,1], u \text{ absolutely continuous.} \tag{2.3}$$

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For each positive integer n and with $\gamma_n = \frac{1}{n}$, define $\phi_n : R^{n+1} \to R$ so that if

$$x = (x_0, x_1, ..., x_n) \in R^{n+1},$$

then

$$\phi_n(x) = \frac{1}{2}\sum_{i=1}^{n}(\frac{x_i - x_{i-1}}{\gamma_n} - \frac{x_i + x_{i-1}}{2})^2. \tag{2.4}$$

Consider first the conventional gradient $\nabla\phi_n$ of ϕ_n. Pick $y \in C^{(3)}$ so that at least one of the following hold:

$$y'(0) - y(0) \neq 0,\ y'(1) - y(1) \neq 0. \tag{2.5}$$

Condition (2.5) amounts to the requirement that $y' - y$ **not** be in the domain of the adjoint of

$$L : Lz = z' - z,\ z \text{ absolutely continuous on } [0,1], \tag{2.6}$$

this adjoint being given by

$$L^t w = \{-(w' + w) : w \text{ absolutely continuous },w(0) = w(1) = 0\}, \tag{2.7}$$

(cf. [56]). Define a sequence of points $\{w^n\}_{n=1}^{\infty}$, $w^n \in R^{n+1}$, $n = 1, 2, ...$, which are taken from y in the sense that for each positive integer n, w^n is the member of R^{n+1} so that

$$w_i^n = y(\frac{i}{n}),\ i = 0, 1, ..., n. \tag{2.8}$$

It will be shown that the measure of worth (2.1) deteriorates badly as the number of grid points approaches ∞. Specifically,

Theorem 2.1.

$$\lim_{n\to\infty} \phi_n(w^n - \delta_n \frac{(\nabla\phi_n)(w^n)}{\phi_n(w^n)}) = 1,$$

where for each positive integer n, δ_n *is chosen optimally in the sense of* (2.2).

This theorem expresses what many have seen in trying to use conventional steepest descent on differential equations. If one makes a definite choice for y with, say $y'(0) - y(0) \neq 0$, then one finds that the gradientsf $(\nabla\phi_n)(w^n)$, even for n quite small, have very large first component relative to all the others (except possibly the last one if $y'(1) - y(1) \neq 0$). This in itself renders $(\nabla\phi_n)(w^n)$ an unpromising object with which to perturb w^n in order that

$$w^{n+1} = w^n - \delta_n(\nabla\phi_n)(w^n)$$

should be a substantially better approximation to a zero of ϕ_n than is w^n (see pictures in Section 2.1).

Proof. Denote $\frac{1}{n}$ by γ_n, $\frac{1}{\gamma_n} + \frac{1}{2}$ by c and $\frac{1}{\gamma_n} - \frac{1}{2}$ by d. Denote

$$Q_n = \begin{pmatrix} -c & d & 0 & \dots & 0 & 0 & 0 \\ 0 & -c & d & 0 & \dots & 0 & 0 \\ 0 & 0 & -c & d & 0 & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & 0 & \dots & 0 & -c & d & 0 \\ 0 & 0 & \dots & 0 & 0 & -c & d \end{pmatrix}$$

Observe that in terms of Q_n,

$$\phi_n(x) = \frac{1}{2}\|Q_n x\|^2,\ x \in R^{n+1}, \tag{2.9}$$

and that if $x, h \in R^{n+1}$ then,

$$\phi_n'(x)h = \langle Q_n h, Q_n x\rangle = \langle h, Q_n^t Q_n x\rangle.$$

Hence

$$\nabla\phi_n = Q_n^t Q_n. \tag{2.10}$$

Thus if $\delta > 0$, $x \in R^{n+1}$ and $Q_n x \neq 0$,

$$\phi_n(x - \delta(\nabla\phi_n)(x)) = \frac{1}{2}\|Q_n(x - \delta Q_n^t Q_n x)\|^2.$$

This expression is a quadratic in δ and has its minimum at

$$\delta_n = \frac{\langle Q_n x, Q_n Q_n^t Q_n x\rangle}{\|Q_n Q_n^t Q_n x\|^2}.$$

In particular,

$$\phi_n \frac{(w^n - \delta_n(\nabla\phi_n)(w^n))}{\phi_n(w^n)} = 1 - \frac{\|Q_n^t g_n\|^4}{\|Q_n Q_n^t g_n\|^2} \cdot \|g_n\|^2$$

where $g_n = Q_n w^n$. Inspection yields that the following limits all exist and are positive:

$$\lim_{n\to\infty} \frac{\|Q_n^t g_n\|^4}{n^4},\ \lim_{n\to\infty} \frac{\|Q_n Q_n^t g_n\|^2}{n^4},\ \lim_{n\to\infty} \frac{1}{n}\|g_n\|^2.$$

It follows that

$$\lim_{n\to\infty} \frac{\phi_n(w^n - \delta_n(\nabla\phi_n)(w^n))}{\phi_n(w^n)} = 1,$$

and the argument is finished. □

Suppose now that ϕ is defined by

$$\phi(z) = \frac{1}{2}\|Lz\|^2, z \in L_2([0,1]),\ z \text{ absolutely continuous.}$$

Suppose in addition that z is $C^{(2)}$ but z is not in the domain of the adjoint (2.7) of L. Then there is no $v \in L_2$ so that

$$\phi'(z)h = \langle h, v\rangle_{L_2([0,1])} \text{ for all } \quad h \in C^2([0,1]).$$

Hence, in a sense, there is nothing that the gradients

$$\{(\nabla\phi_n)(w^n)\}_{n=1}^{\infty}$$

are approximating. One should expect really bad numerical performance of these gradients (and this expectation is met).

This example represents something common for differential equations. Sobolev gradients give an organized way to modify poorly performing gradients in order to obtain gradients with good numerical and analytical properties.

A construction of a Sobolev gradient is now given, which for a given positive integer n, corresponds to the ordinary one above. The theorem to follow makes a comparison with the result of Theorem 2.1. Choose a positive integer n. A second gradient. to be denoted by $\nabla_{S_n}\phi$, is taken with respect to a second norm on R^{n+1}. This norm is defined by a finite dimensional version of a Sobolev norm:

$$\|x\|_{S_n} = [\sum_{i=1}^{n}(\frac{x_i - x_{i-1}}{\gamma_n})^2 + (\frac{x_i + x_{i-1}}{2})^2)]^{1/2},\ x = (x_0, x_2, \ldots, x_n) \in R^{n+1}. \tag{2.11}$$

It is easy to see that this norm carries with it an inner product

$$\langle\ \cdot, \cdot\rangle_{S_n}$$

on R^{n+1} which is related to the standard inner product $\langle\ ,\ \rangle$ on R^{n+1} as follows:

$$\langle x, y\rangle_{S_n} = \langle A_n x, y\rangle,$$

where if $x = (x_0, x_1, ..., x_n)$, then

$$A_n x = z$$

so that

$$z_0 = \frac{1}{2}(c^2 + d^2)x_0 - cdx_1,$$
$$z_i = -cdx_{i-1} + (c^2 + d^2)x_i - cdx_{i+1},\ i = 1, ..., n-1,$$
$$z_n = -cdx_{n-1} + \frac{1}{2}(c^2 + d^2)x_n,$$

in which c, d are as in Theorem 2.1. Accordingly, using (1.3), the gradient $\nabla_{S_n}\phi_n$ of ϕ_n is

$$(\nabla_{S_n}\phi_n)(x) = A_n^{-1}(\nabla\phi_n)(x). \tag{2.12}$$

In contrast to Theorem 2.1 we have

Theorem 2.2. *If $x \in R^{n+1}$ then*

$$\phi_n(x - \delta_n(\nabla_{S_n}\phi_n)(x)) \leq \frac{1}{9}\phi_n(x),\ n = 1, 2, \ldots,$$

where for each n, δ_n is chosen optimally.

This indicates that $\nabla_{S_n}\phi_n$ performs much better numerically than does $\nabla\phi_n$.

Lemma 2.3. *Suppose n is a positive integer, $\lambda > 0$, $v \in R^n$, $v \neq 0$. Suppose also that $M \in L(R^n, R^n)$ is so that $Mv = \lambda v$ and $Mx = x$ if $\langle x, v\rangle = 0$. Then*

$$\frac{\langle My, y\rangle^2}{(\|My\|^2\|y\|^2)} \geq \frac{4\lambda}{(1+\lambda)^2} \in R^n, y \neq 0.$$

Proof. Pick $y \in R^n$, $y \neq 0$ and write $y = x + r$ where r is a multiple of v and $\langle x, r\rangle = 0$. Then

$$\begin{aligned}\frac{\langle My, y\rangle^2}{\|My\|^2\|y\|^2} &= \frac{\langle x + \lambda r, x + r\rangle}{(\|x + \lambda r\|^2\|x + r\|^2)} \\ &= \frac{(\|x\|^2 + \lambda\|r\|^2)^2}{(\|x\|^2 + \lambda^2\|r\|^2)(\|x\|^2 + \|r\|^2))} \\ &= \frac{(\sin^2\theta + \lambda\cos^2\theta)^2}{(\sin^2\theta + \lambda^2\cos^2\theta)},\end{aligned} \tag{2.13}$$

where

$$\sin^2\theta = \frac{\|x\|^2}{(\|x\|^2 + \|r\|^2)},\ \cos^2\theta = \frac{\|r\|^2}{(\|x\|^2 + \|r\|^2)}.$$

Expression (2.13) is seen to have its minimum for $\cos^2\theta = \frac{1}{1+\lambda}$. The lemma readily follows. □

Proof. (Theorem 2.2). Denote $Q_n A_n^{-1} Q_n^t$ by M_n. Using (2.9), (2.10), (2.12), for $x \in R^{n+1}$, $\delta \geq 0$,

$$\phi_n(x - \delta(\nabla_{S_n}\phi_n)(x)) = \|g\|^2 - 2\delta\langle g, M_n g\rangle + \delta^2\|M_n g\|^2,$$

where $g = Q_n x$. This expression is minimized by choosing

$$\delta = \delta_n = \frac{\langle g, M_n g\rangle}{\|M_n g\|^2},$$

so that with this choice of δ,

$$\frac{\phi_n(x - \delta_n(\nabla_{S_n}\phi_n)(x))}{\phi_n(x)} = 1 - \frac{\langle g, M_n g\rangle^2}{(\|M_n g\|^2\|g\|^2)}.$$

To get an expression for $M_n g$, first calculate $u = A_n^{-1} Q_n^t g$. To accomplish this solve

$$A_n u = Q_n^t g \tag{2.14}$$

for $u = (u_0, u_1, ..., u_n)$. Writing $(g_1, ..., g_n)$ for g, (2.14) becomes the system

$$\frac{1}{2}(c^2 + d^2)u_0 - cdu_1 = -cg_1, \tag{2.15}$$
$$-cdu_{i-1} + (c^2 + d^2)u_i - cdu_{i+1} = dg_i - cg_{i+1},\ i = 1, ..., n-1,$$
$$-cdu_{n-1} + \frac{1}{2}(c^2 + d^2)u_n = dg_n.$$

From equations $1, ..., n-1$ it follows, using standard difference equation methods, that there must be α and β so that

$$u_0 = \alpha r^0 + \beta s^0$$

$$u_i = \alpha r^i + \beta s^i + \frac{1}{d}\sum_{k=1}^{i} r^{i-k} g_k,\ i = 1, ..., n, \tag{2.16}$$

where $r = \frac{c}{d}$, $s = \frac{d}{c}$. The first equation of (2.15) implies that $\alpha = \beta$. The last equation in (2.15) may then be solved for α, leaving

$$u_0 = -\eta(r^0 + s^0)u_i = -\eta(r^i + s^i) + \frac{1}{d}(\sum_{k=1}^{i} r^{i-k} g_k), i = 1, ..., n, \tag{2.17}$$

where

$$\eta = \frac{\sum_{k=1}^{n} r^{n-k} g_k}{d(r^n - s^n)}.$$

Note that $M_n g = Q_n u$. After some simplification of (2.17),

$$M_n g = \langle g, z^{(n)} \rangle z^{(n)} + g,$$

where $z^{(n)} = (z_1, ..., z_n)$ is defined by

$$z_i = (\sum_{k=0}^{n-1} s^{2k})^{-1/2} s^{i-1},\ i = 1, ..., n.$$

Note that $\|z^{(n)}\| = 1$ and that M_n satisfies the conditions of Lemma 2.3 with $\lambda = 2$. Accordingly,

$$1 - \frac{\langle g, M_n g \rangle^2}{\|M_n g\|^2 \|g\|^2} \leq 1 - 4\frac{\lambda}{(1+\lambda)^2} = \frac{(\lambda-1)^2}{(\lambda+1)^2} = \frac{1}{9}.$$

Hence

$$\frac{\phi_n(x - \delta_n(\nabla_{A_n}\phi_n)(x)}{\phi_n(x)} \leq \frac{1}{9},$$

and the argument is complete. □

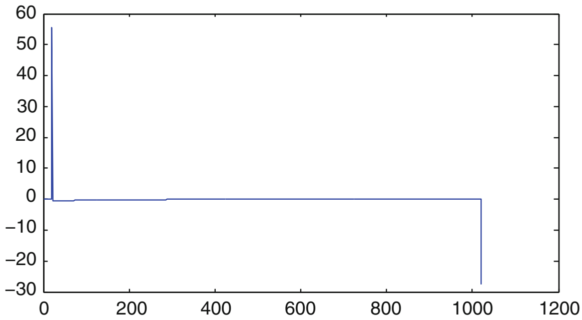
The above follows an argument in [157] for a slightly different case.

The inequality in Theorem 2.2 implies a good rate of convergence for discrete steepest descent since it indicates that the ratio of the norm of a new residual and the norm of the corresponding old residual is no more than 1/3. One may see that Theorem 2.2 can be extended by continuity to a function space setting. No such extension of Theorem 2.1 seems possible. Actual programming of the process in Theorem 2.1 leads to a very slowly converging iteration. The number of steps required to reach a fixed accuracy increases very fast as n increases with perhaps 500,000 iterations required for $n = 100$. By contrast, the process in Theorem 2.2 requires about 7 steps, independently of the choice of n. A computer code connected with Theorem 2.2 is given in Chapter 24. The following section shows some results from that code.

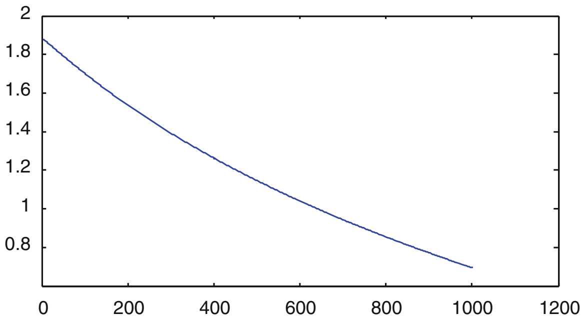
2.1 A Graphical Comparison Between Two Gradients

Graphs of gradients (2.4) and (2.12) for $n = 1000$ follow. For the function v : defined by (almost any function would do here), follow in Figure 2.1

$$v(t) = \frac{1}{1+t},\ t \in [0, 1],$$



(a) Ordinary Gradient



(b) Sobolev Gradient

Fig. 2.1 Ordinary and Sobolev Gradients Compared

a starting value u for discrete steepest descent was taken:

$$u(k) = v\left(\frac{k-1}{n}\right),\ k = 1, 2, \ldots, n+1.$$

The first graph is the resulting ordinary gradient, actually a plot of

$$f' * f * u$$

in the MatLab code in Figure 24.1.

The second graph gives the corresponding Sobolev gradient, actually g in that code. The first graph was shifted to the right 20 units so as distinguish between the vertical axis and the leftmost portion of the graph. Note that the ordinary gradient is very large at the left and right endpoints and nearly (but not quite) zero in between. Such a gradient is not a good candidate to multiply by a positive number and then subtract from u in order to get significantly closer to a solution to the underlying differential equation.

The Sobolev gradient is of a better nature. In (2.12) one sees how these two gradients are related. What is represented here is a common feature of how Sobolev gradients for differential equations relate to corresponding ordinary gradients. The embedding operator A_n^{-1} (see Chapter 5) supplies a relevant preconditioner (see Chapter 29).

The closest thing to an ordinary gradient for the problem in this chapter is an everywhere discontinuous, only densely defined transformation. This is what, in effect, ordinary gradients of corresponding discrete problems are attempting, with essentially no success, to approximate. By contrast, it will be seen later that the corresponding Sobolev gradient in function space is a linear and continuous, everywhere defined transformation. The pathology of the first compared to the benign, but efficient, nature of the second, has its counterpart in corresponding discrete versions. This is a reflection of my:

First Law of Numerical Analysis:
Analytical and Numerical Difficulties Always Come Paired.

Chapter 3
Continuous Steepest Descent in Hilbert Space: Linear Case

This chapter deals with continuous steepest descent for linear operator equations in Hilbert spaces.

Suppose that each of H and K is a Hilbert space and that

$$G \in L(H,K),\ g \in K \text{ and } Fx = Gx - g,\ x \in H.$$

The following shows that if there is a solution v to $Fv = 0$, then a solution may be found by means of continuous steepest descent.

The adjoint G^* of G is the member of $L(K,H)$ so that

$$\langle Gx, y\rangle_K = \langle x, G^* y\rangle_H,\ x \in H, y \in K.$$

Theorem 3.1. *Suppose there is $v \in H$ so that $Gv = g$ and*

$$\phi(y) = \|Gy - g\|_K^2/2,\ y \in H.$$

Suppose also that $x \in H$ and z is the function on $[0,\infty)$ so that

$$z(0) = x,\ z'(t) = -(\nabla\phi)(z(t)),\ t \geq 0. \tag{3.1}$$

Then $u = \lim_{t\to\infty} z(t)$ exists and $Gu = g$.

Proof. First note that

$$\phi'(y)h = \langle Gh, Gy - g\rangle_K = \langle h, G^*(Gy - g)\rangle_H$$

so that

$$(\nabla\phi)(y) = G^*(Gy - g),\ y, h \in H. \tag{3.2}$$

Restating (3.1),

$$z(0) = x,\ z'(t) = -G^*Gz(t) + G^*g,\ t \geq 0.$$

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_3,

From elementary ordinary differential equations in a Banach space there is the following 'variation of parameters' formula:

$$z(t) = \exp(-tG^*G)x + \int_0^t \exp(-(t-s)G^*G)G^*g\ ds,\ t \geq 0. \tag{3.3}$$

By hypothesis, v is such that $Gv = g$. Replacing g in the preceding by Gv and using the fact that

$$\int_0^t \exp(-(t-s)G^*G)G^*Gv\ ds = \exp(-(t-s)G^*G)v\,\Big|_{s=0}^{s=t} = v - \exp(-tG^*G)v$$

it follows that

$$z(t) = \exp(-tG^*G)x + v - \exp(-tG^*G)v.$$

Now since G^*G is symmetric and nonnegative, $\exp(-tG^*G)$ converges strongly (that is, pointwise), as $t \to \infty$, to the orthogonal projection P onto the null space of G (see the discussion of the spectral theorem in [204], Chap. VII). Accordingly,

$$u \equiv \lim_{t\to\infty} z(t) = Px + v - Pv \text{ exists.}$$

But then

$$Gu = GPx + Gv - GPv = Gv = g$$

since $Px, Pv \in N(G)$. □

Notice that abstract existence of a solution v to $Gv = g$ leads to a concrete function z whose asymptotic limit is a solution u to

$$Gu = g.$$

A reader might refer to [125] in connection with these problems. In case g is not in the range of G there is the following:

Theorem 3.2. *Suppose $G \in L(H, K)$, $g \in K$, $x \in H$ and z satisfies (3.1). Then*

$$\lim_{t\to\infty} Gz(t) = g - Qg$$

where Q is the orthogonal projection of K onto $R(G)^\perp$.

Proof. Using (3.3),

$$\begin{aligned} Gz(t) &= G(\exp(-tG^*G)x) + G(\int_0^t \exp(-(t-s)G^*G)G^*g\ ds),\ t \geq 0 \\ &= \exp(-tGG^*)Gx + \int_0^t \exp(-(t-s)GG^*)GG^*g\ ds \end{aligned}$$

$$= \exp(-tGG^*)Gx + \exp(-(t-s)GG^*)g \,\Big|_{s=0}^{s=t}$$
$$= \exp(-tGG^*)Gx + g - \exp(-tGG^*)g \to g - Qg \text{ as } t \to \infty,$$

since $\exp(-tGG^*)$ converges strongly to Q, the orthogonal projection of K onto $N(G^*) = R(G)^\perp$, as $t \to \infty$ ($N(G^*)$ means the null space of G^*, $R(G)$ means the range of G). □

The following characterizes the solution u obtained in Theorem 3.1:

Theorem 3.3. *Under the hypothesis of Theorem 3.1, if $x \in H$ and z is the function from $[0,\infty)$ to H so that (3.1) holds, then $u \equiv \lim_{t\to\infty} z(t)$ has the property that if $y \in H, y \neq u$ and $Gy = g$, then*

$$\|u - z(t)\|_H < \|y - z(t)\|_H,\ t \geq 0.$$

Proof. Suppose $w \in H$ and $Gw = g$. For u as in the argument for Theorem 3.1, notice that $u - w \in N(G)$ and

$$x - u = (I - P)(x - v).$$

Hence $\langle x-u, u-w\rangle_H = 0$ since $I - P$ is the orthogonal projection onto $N(G)^\perp$. Consequently

$$\|x - w\|_H^2 = \|x - u\|_H^2 + \|u - w\|^2,$$

and so u is the nearest element q to x which has the property that $Gq = g$. Now if $t \geq 0$, then

$$x - z(t) = (I - \exp(-t^*GG))(x - v).$$

Since

$$P\exp(-tG^*G) = P,$$

it follows that

$$P(x - z(t)) = 0,$$

and hence u is also the nearest element to x which has the property that $Gu = g$. □

Another way to express the intent of Theorem 3.2 is to say that P, the orthogonal projection onto $N(G)$, provides an invariant for steepest descent generated by $-\nabla\phi$ in the sense that

$$Px = P(z(t)),\ t \geq 0.$$

An invariant (or a set of invariants) for steepest descent in nonlinear cases would be very interesting. More about this problem will be indicated in Chapters 19 and 20.

Chapter 4
Continuous Steepest Descent in Hilbert Space: Nonlinear Case

Denote by H a real Hilbert space and suppose that ϕ is a $C^{(1)}$ real-valued function with locally lipschitzian gradient on all of H. For this chapter, denote by $\nabla\phi$ the function on H so that if $x \in H$, then

$$\phi'(x)h = \langle h, (\nabla\phi)(x)\rangle_H,\ h \in H,$$

where ϕ' denotes the Fréchet derivative of ϕ. Here are sought zeros of $\nabla\phi$ by means of continuous steepest descent, *i.e.*, $u \in H$ is sought so that

$$u = \lim_{t\to\infty} z(t) \text{ exists and } (\nabla\phi)(u) = 0, \tag{4.1}$$

where z satisfies (4.2). It will be seen that in many important instances, a zero of $\nabla\phi$ is also a zero of ϕ. In later chapters related results for continuous Newton's method are explored.

4.1 Global Existence

First we establish global existence for steepest descent in this setting.

Theorem 4.1. *Suppose that ϕ is non-negative $C^{(1)}$ function on H which has a locally lipschitzian gradient. If $x \in H$, there is a unique function z from $[0,\infty)$ to H such that*

$$z(0) = x,\ z'(t) = -(\nabla\phi)(z(t)),\ t \geq 0. \tag{4.2}$$

Proof. From (0.1), generalized to Banach spaces in a straightforward way, there is $d_0 > 0$ so that the equation in (4.2) has a solution on $[0, d_0)$. Suppose that the set of all such numbers d_0 is bounded and denote by d its least upper bound.

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_4,

Denote by z the solution to the equation in (4.2) on $[0, d)$. It will be shown first that $\lim_{t\to d-} z(t)$ exists. To this end note that if $0 \le a < b < d$ then

$$\|z(b) - z(a)\|_H^2 = \| \int_a^b z'\|_H^2 \le (\int_a^b \|z'\|_H)^2 \le (b-a)\int_a^b \|z'\|_H^2. \tag{4.3}$$

Note that if $t \in [0, d)$, then

$$\phi(z)'(t) = \phi'(z(t))z'(t) = \langle z'(t), (\nabla\phi)(z(t)\rangle_H = -\|(\nabla\phi)(z(t))\|_H^2 \tag{4.4}$$

so

$$\phi(z(b)) - \phi(z(a)) = \int_a^b \phi(z)' = -\int_a^b \|z'\|_H^2.$$

Hence,

$$\int_a^b \|z'\|_H^2 \le \phi(z(a)),\ 0 \le a < b < d. \tag{4.5}$$

Using (4.3) and (4.5),

$$\|z(b) - z(a)\| \le ((b-a)\int_a^b \|z'\|_H^2)^{\frac{1}{2}} \le (d\phi(a))^{\frac{1}{2}},\ a \le b < d.$$

But this implies that $\int_a^{d-} \|z'\|_H$ exists and so $q \equiv \lim_{t\to d-} z(t)$ exists. But again, from (0.1), there is $c > d$ for which there is a function y on $[d, c)$ such that

$$y(d) = q,\ y'(t) = -(\nabla\phi)(y(t)),\ t \in [d, c).$$

The function w on $[0, c)$ so that

$$w(t) = z(t),\ t \in [0, d),\ w(d) = q,\ w(t) = y(t),\ t \in (d, c),$$

satisfies

$$w(0) = x, w'(t) = -(\nabla\phi)(w(t)),\ t \in [0, c),$$

contradicting the nature of d since $d < c$. Hence there is a solution to (4.2) on $[0, \infty)$. Uniqueness follows from (0.1). □

A useful observation is:

Theorem 4.2. *Under the hypothesis of Theorem 4.1, if*

$$u = \lim_{t\to\infty} z(t) \tag{4.6}$$

exists, then

$$(\nabla\phi)(u) = 0.$$

Proof. For z satisfying (4.2),

$$(\phi(z))' = -\|(\nabla\phi)(z)\|^2,$$

as in the argument for Theorem 4.1. Then

$$\phi(z(t)) - \phi(z(0)) = -\int_0^t \|(\nabla\phi)(z)\|^2$$

and so

$$\phi(z(0)) \geq \int_0^t \|(\nabla\phi)(z)\|^2,\ t \geq 0.$$

Assuming $(\nabla\phi)(u) \neq 0$ leads to a contradiction. □

See [18] for another discussion of steepest descent in Hilbert spaces.

A function ϕ as in the hypothesis of Theorem 4.1 generates a one parameter semigroup of transformations on H. Specifically, define T_ϕ so that if $s \geq 0$, then $T_\phi(s)$ is the transformation from H to H such that

$$T_\phi(s)x = z(s),\ \text{where}\ \ z \text{ satisfies (4.2)}.$$

Theorem 4.3. *$T_\phi(t)T_\phi(s) = T_\phi(t+s)$, $t, s \geq 0$ where $T_\phi(t)T_\phi(s)$ indicates composition of the transformations $T_\phi(t)$ and $T_\phi(s)$.*

Proof. Suppose $x \in H$ and $s > 0$. Define z satisfying (4.2) and define y so that

$$y(s) = T_\phi(s)x,\ y'(t) = -(\nabla\phi)(y(t)),$$

$t \geq s$. Since $y(s) = z(s)$ and y, z satisfy the same differential equation on $[s, \infty)$, by uniqueness it follows that $y(t) = z(t),\ t \geq s$ and hence the truth of the theorem. □

Note that the assumption that ϕ is bounded below is sufficient for similar results as those above.

4.2 Gradient Inequality

Note that the argument for Theorem 4.1 yields that

$$\int_0^\infty \|(\nabla\phi)(z)\|_H^2 < \infty \tag{4.7}$$

under the hypothesis of that theorem. Now the conclusion

$$\int_0^\infty \|(\nabla\phi)(z)\|_H < \infty \tag{4.8}$$

implies, as in the argument for Theorem 4.1, that $\lim_{t\to\infty} z(t)$ exists. Clearly (4.7) does not imply (4.8). For an example, take $\phi(x) = e^{-x}$, $x \in R$. Note also that under the hypothesis of Theorem 4.1 one has

$$\{\phi(z(t))\ :\ t \geq 0\} \text{ is bounded,} \tag{4.9}$$

since $\phi(z(t)) \leq \phi(x), t \geq 0$. Following are some propositions which lead to the conclusion (4.8).

Definition. Suppose $\theta \in (0,1)$. ϕ is said to satisfy a gradient inequality on $\Omega \subset H$ with exponent θ provided there is $c_0 > 0$ such that

$$\|(\nabla\phi)(x)\|_H \geq c_0\phi(x)^\theta,\ x \in \Omega. \tag{4.10}$$

In case each of H, K is a Hilbert space, $\theta \in (0,1)$, $F : H \to K$ is a C^1 function and

$$\phi(x) = \frac{1}{2}\|F(x)\|_K^2,\ x \in H, \tag{4.11}$$

then a gradient inequality for ϕ on a subset Ω with exponent $\frac{1}{2}$ of ϕ would read as follows: there is $c > 0$, so that

$$\|(\nabla\phi)(x)\|_H \geq c\|F(x)\|_K,\ x \in \Omega. \tag{4.12}$$

Note that for $\theta = \frac{1}{2}$, c in (4.12) and c in (4.10) differ only by a factor of $\sqrt{2}$.

Saying simply that ϕ satisfies a gradient inequality will mean that ϕ satsfies a gradient inequality with exponent $\frac{1}{2}$.

It will be seen that this condition gives compactness in some instances and leads to (4.1) holding (Theorems 4.4, 4.5, 4.8, 4.9, 4.11 and Lemma 4.7.)

Theorem 4.4. *Suppose ϕ is a nonnegative $C^{(1)}$ function with locally lipschitzian gradient on $\Omega \subset H$ and ϕ satisfies (4.10). If $x \in \Omega$ and z satisfies (4.2) then (4.1) holds provided that $R(z) \subset \Omega$.*

Proof. Suppose z satisfies (4.2), (4.10) holds on Ω and $R(z) \subset \Omega$. Note that if $(\nabla\phi)(x) = 0$, then the conclusion holds. Suppose that $(\nabla\phi)(x) \neq 0$ and note that then $(\nabla\phi)(z(t)) \neq 0$ for all $t \geq 0$ since if $(\nabla\phi)(z(t_0) = 0$ for some $t_0 \geq 0$, then the function w on $[0,\infty)$ defined by $w(t) = z(t_0)$, $t \geq 0$, would satisfy $w' = -(\nabla\phi)(w)$ and $w(t_0) = z(t_0)$, the same conditions as z; but $z \neq w$ and so uniqueness would be violated. Now by (4.4),

$$\phi(z)' = -\|(\nabla\phi)(z)\|_H^2$$

and so, using (4.10)

$$(\phi(z))'(t) = -c\|z'(t)\|_H\|(\nabla\phi)(t)\|_H,\ t \geq 0.$$

and hence

$$((\phi(z))'(t) \leq -c\|z'(t)\|_H \phi(z(t))^\theta,\ t \geq 0.$$

Thus

$$\frac{(\phi(z))'(t)}{\phi(z(t))^\theta} \leq -c\|z'(t)\|_H,\ t \geq 0.$$

Accordingly,

$$\frac{1}{1-\theta}(\phi(z(t))^{1-\theta} - (\phi(z(0))^{1-\theta}) \leq -c\int_0^t \|z'\|_H,\ t \geq 0,$$

and therefore

$$\int_0^t \|z'\|_H \leq \frac{1}{c(1-\theta)}((\phi(z(0))^{1-\theta},\ t \geq 0. \tag{4.13}$$

Thus

$$u = \lim_{t\to\infty} z(t)$$

exists. Consequently,

$$(\nabla\phi)(u) = 0$$

and so

$$\phi(u) = 0$$

due to (4.10). □

The following theorem gives an instance in which boundedness of z satisfying (4.2) is assured. This result is a point of departure for a related Nash-Moser inverse function theorem result *via* continuous Newton's method (Chapter 9). This is a clear instance for which one can see how a gradient inequality induces compactness.

Theorem 4.5. *Suppose that each of H and K is a Hilbert space, $r, c > 0$, $x \in H$, $F : B_r(x) \to K$ is a C^1 function,*

$$\phi(y) = \frac{1}{2}\|F(y)\|_K^2,\ y \in B_r(x), \tag{4.14}$$

and ϕ has a locally lipschitzian gradient on $B_r(x)$. Suppose also that

$$\|(\nabla\phi)(y)\|_H \geq c\|F(y)\|_H,\ y \in B_r(x). \tag{4.15}$$

If

$$rc \leq 1,$$

then $z : [0, \infty) \to B_r(x)$ *satisfying*

$$z(0) = x, \ z'(t) = -(\nabla\phi)(z(t)), \ t \geq 0$$

satisfies also

$$u = \lim_{t\to\infty} z(t)$$

and hence

$$F(u) = 0.$$

Proof. Taking into account the comment following (4.12), (4.13) translates, for the choice of $\theta = \frac{1}{2}$, to

$$\int_0^t \|z'\|_H \leq \frac{1}{c}\|F(x)\|_K, \ t \geq 0,$$

implying that

$$\int_0^t \|z'\|_H \leq r, \ t \geq 0,$$

since by hypothesis, $\|F(x)\| \leq rc$. Thus, $z(t)$ is unable to escape $B_r(x)$, even as $t \to \infty$, and so Theorem 4.4 gives the conclusion. □

A zero finding result that does not use a gradient inequality is the following (see [97]):

Theorem 4.6. *Suppose that* H *is a Hilbert space,* Q *is a real valued* C^1 *function on* H *which has a locally lipschitzian gradient* ∇Q *and*

$$\phi(x) = \frac{1}{2}\|x\|_H^2 + Q(x), \ x \in H.$$

Suppose also that ϕ *is coercive,* $x \in H$ *and* z *satisfies* (4.2)*. If* $\nabla(Q)$ *is compact, then* ϕ *has an* ω*-limit point* u *and* $(\nabla\phi)(u) = 0$.

ϕ is said to be coercive if

$$\lim_{\|x\|_H\to\infty} \phi(x) = \infty.$$

Proof. Suppose that z satisfies (4.2) and note that due to (4.7), there is $\{t_k\}_{k=1}^{\infty}$ so that

$$\lim_{t_k\to\infty} (\nabla\phi)(z(t_k)) = 0.$$

Furthermore, this sequence, due to the compactness assumption on ∇Q, has a subsequence $\{t_{k_j}\}_{j=1}^{\infty}$ so that

$$w = \lim_{j\to\infty} (\nabla Q)(z(t_{k_j}))$$

exists. Since

$$(\nabla\phi)(x) = x + (\nabla Q)(x),\ x \in H,$$

it follows that

$$u = \lim_{j\to\infty} z(t_{k_j})$$

exists and hence $(\nabla\phi)(u) = 0$. □

The following lemma leads to short arguments for Theorems 4.8 and 4.9.

Lemma 4.7. *Suppose ϕ is a nonnegative C^1 function on H which has a locally lipschitzian derivative, $c > 0$ and Ω is an open subset of H so that (4.10) holds. Suppose that $x \in H$ and z satisfies (4.2). Then there do not exist $\epsilon > 0$ and sequences*

$$\{s_i\}_{i=1}^{\infty}, \{r_i\}_{i=1}^{\infty}$$

so that $\{[s_i, r_i]\}_{i=1}^{\infty}$ is a sequence of pairwise disjoint intervals with the property that

1. $s_n, r_n \to \infty$ *as* $n \to \infty$,
2. $s_i < r_i < s_{i+1}$,
3. $\|z(r_i) - z(s_i)\|_H \geq \epsilon$
4. $z(t) \in \Omega$ *if* $t \in [s_i, t_i]$, *for* $i = 1, 2, \ldots$.

Proof. Suppose that the hypothesis holds but that the conclusion does not. Denote by ϵ a positive number and by

$$\{s_i\}_{i=1}^{\infty}, \{r_i\}_{i=1}^{\infty}$$

sequences so that $\{[r_i, s_i]\}_{i=1}^{\infty}$ is a sequence of pairwise disjoint intervals so that (1)-(4) hold. Note that $(\nabla\phi)(z(t)) \neq 0$ for $t \geq 0$ since if not then $(\nabla\phi)(z(t)) = 0$ for all $t \geq 0$ and hence z is constant and consequently, (3) is violated. Now for each positive integer i,

$$\epsilon^2 \leq \|z(r_i) - z(s_i)\|_H^2 = \|\int_{s_i}^{r_i} z'\|_H^2$$
$$\leq (\int_{s_i}^{r_i} \|z'\|_H)^2 \leq (r_i - s_i)\int_{s_i}^{r_i} \|z'\|_H^2.$$

As in the proof for Theorem 4.1, if $0 \leq a < b$,

$$\phi(z(a)) = \phi(z(b)) + \int_a^b \|z'\|_H^2.$$

Hence $\int_0^\infty \|z'\|_H^2$ exists and therefore

$$\lim_{i\to\infty} \int_{s_i}^{r_i} \|z'\|_H^2 = 0.$$

Consequently, $\lim_{i\to\infty}(r_i - s_i) = \infty$ since

$$\epsilon^2 \le (r_i - s_i)\int_{s_i}^{r_i} \|z'\|_H^2,\ i = 1, 2, \ldots.$$

Since

$$\phi(z)'(t) = -\|(\nabla\phi)(z(t)\|_H^2 \le -c^2\phi(z(t)), t \ge 0,$$

it follows that

$$\phi(z)'(t)/\phi(z(t)) \le -c^2,\ t \ge 0$$

and so for each positive integer i,

$$\phi(z(t)) \le \phi(z(s_i))\exp(-c^2(t - s_i)),\ t \in [s_i, r_i],$$

and in particular,

$$\phi(z(r_i)) \le \phi(z(s_i))\exp(-c^2(r_i - s_i)).$$

Therefore, since $\phi(z(r_i)) \ge \phi(z(s_{i+1})),\ i = 1, 2, \ldots,$ it follows that

$$\lim_{i\to\infty}\phi(z(s_i)) = 0.$$

Denote by i a positive integer so that $r_i - s_i > 1$, denote $[r_i - s_i]$ by k and denote $s_i, s_i + 1, ..., s_i + k, r_i$ by $q_0, q_1, ..., q_{k+1}$. Then

$$\begin{aligned}
&\epsilon \le \|z(r_i) - z(s_i)\|_H \le \sum_{j=0}^{k}\|z(q_{j+1}) - z(q_j)\|_H \le \sum_{j=0}^{k}\int_{s_i+j}^{s_i+j+1}\|z'\|_H \\
&\le \sum_{j=0}^{k}(\int_{s_i+j}^{s_i+j+1}\|z'\|_H^2)^{1/2} = \sum_{j=0}^{k}(\phi(z(s_i + j)) - \phi(z(s_i + j + 1)))^{1/2} \\
&\le \sum_{j=0}^{k}\phi(z(s_i + j))^{1/2} \le \sum_{j=0}^{k}(\phi(z(s_i))\exp(-c^2 j)^{\frac{1}{2}} \\
&= (\phi(z(s_i))\sum_{j=0}^{k}\exp(-c^2 j))^{\frac{1}{2}} \le \phi(z(s_i))^{\frac{1}{2}}\sum_{j=0}^{k}\exp(-jc^2/2) \\
&\le \phi(z(s_i))^{\frac{1}{2}}(1 - \exp(-c^2/2))^{-1}
\end{aligned}$$

since

$$\phi(z(a + 1)) \le \phi(z(a))\exp(-c^2), a = s_i, s_i + 1, \ldots s_i + k - 1$$

under our hypothesis. But since

$$\phi(z(s_i)) \to 0 \text{ as } i \to \infty$$

one arrives at a contradiction. □

The following rules out some conceivable alternatives:

Theorem 4.8. *Suppose that ϕ is a nonnegative $C^{(2)}$ function on all of H which satisfies (4.10) for every bounded subset Ω of H. If z satisfies (4.2) then either*

$$(i) \ \ (4.1) \text{ holds, or else}$$
$$(ii) \ \ \lim_{t\to\infty} \|z(t)\|_H = \infty.$$

Proof. Suppose that $x \in H$, z satisfies (4.2) and (4.10) holds for every bounded subset Ω of H. Suppose furthermore that $R(z)$ is not bounded but nevertheless does not satisfy (ii) of the theorem. Then there are $r, s > 0$ so that $0 < s < r$, and two unbounded increasing sequences $\{r_i\}_{i=1}^{\infty}, \{s_i\}_{i=1}^{\infty}$ so that

$$\begin{aligned}
&s_i < r_i < s_{i+1},\\
&\|z(s_i)\|_H = s, \|z(r_i)\|_H = r,\\
&s \le \|z(t)\|_H \le r,\ t \in [s_i, r_i],\ i = 1, 2, \dots.
\end{aligned}$$

But by the Lemma 4.7, this is impossible and the theorem is established. □

A similar phenomenon has been indicated in [11] for semigroups related to monotone operators.

Theorem 4.9. *Under the hypothesis of Theorem 4.8, suppose that $x \in H$ and z satisfies (4.2). Suppose also that u is an ω-limit point of z, i.e.,*

$$u = \lim_{i\to\infty} z(t_i)$$

for some increasing unbounded sequence of positive numbers $\{t_i\}_{i=1}^{\infty}$. Then (4.1) holds.

Proof. If z has an ω-limit point then (ii) of Theorem 4.8 can not hold and hence (i) must hold. □

Without imposing a gradient inequality condition one has the following:

Theorem 4.10. *Suppose that ϕ is a nonnegaitve C^1 function on the Hilbert space H, $\nabla\phi$ is locally lipschitzian, z satisfies (4.2) and z has an $\omega-$limit point u. Then $(\nabla\phi)(u) = 0$.*

Proof. Suppose u is an ω-limit point of z so that $(\nabla\phi)(u) \neq 0$. Then it is not the case that (4.1) holds since if it did, $(\nabla\phi)(u) = 0$. Denote by each of r_0, M a positive number so that

$$\|(\nabla\phi)(x)\| \geq M\phi(x)^{\frac{1}{2}}, \ \text{ if } \|x - w\|_H \leq r_0.$$

Denote by r a positive number satisfying $2r \leq r_0$ so that if $q > 0$ there are s, t so that

$$q < s < t, \|z(s) - w\|_H < r, \|z(t) - w\| < 2r \text{ and } \|z(t) - z(s)\|_H > r.$$

Denote by $\{r_k\}_{k=0}^{\infty}, \{s_k\}_{k=0}^{\infty}$ two sequences of positive numbers converging to infinity so that

- $s_k < r_k < s_k$,
- $\|z(s_k) - w\|_H \leq r$,
- $r < \|z(r_k) - z(s_k)\|_H$,
- $\|z(r_k) - w\|_H < 2r_0, \ k = 1, 2, \ldots.$

But these items contradict the truth of Lemma 4.7, and so an argument is finished. □

A reader is reminded of the Palais-Smale condition (see [175]) on ϕ : ϕ satisfies the Palais-Smale condition provided it is true that if $\{x_i\}_{i=1}^{\infty}$ is a sequence for which $\lim_{i\to\infty}(\nabla\phi)(x_i) = 0$ and $\{\phi(x_i)\}_{i=1}^{\infty}$ is bounded, then $\{x_i\}_{i=1}^{\infty}$ has a convergent subsequence. This leads to the following:

Theorem 4.11. *Suppose that ϕ is a nonnegative C^1 function on H which has a locally lipschitzian derivative, satisfies the Palais-Smale condition and also satisfies* (4.10) *for every bounded subset Ω of H. Then* (4.1) *holds.*

Proof. Since by the proof of Theorem 4.1, (4.7) holds, it follows that there is an unbounded increasing sequence $\{t_i\}_{i=1}^{\infty}$ of positive numbers such that

$$\lim_{i\to\infty}(\nabla\phi)(z(t_i)) = 0.$$

Note also that

$$\phi(x) \geq \phi(z(t)) \geq 0, \ t \geq 0$$

holds. It follows from the (PS) condition that there is an increasing sequence $\{n_i\}_{i=1}^{\infty}$ of positive integers such that $\{z(t_{n_i})\}_{i=1}^{\infty}$ converges. But this rules out (ii) of Theorem 4.8 so that (i) of that theorem must hold. □

Note that in the above, the full strength of the (PS) condition is not used. Requiring that '$\{x_i\}_{i=1}^{\infty}$ has a bounded subsequence' is sufficient for the purpose of Theorem 4.11.

Suppose now that K is a second real Hilbert space and that F is a $C^{(2)}$ function from H to K. Define ϕ by

$$\phi(x) = \frac{1}{2}\|F(x)\|_K^2,\ x \in H. \tag{4.16}$$

In this case

$$\phi'(x)h = \langle F'(x)h, F(x)\rangle_K = \langle h, F'(x)^* F(x)\rangle_H,\ x, h, \in H,$$

so that

$$(\nabla\phi)(x) = F'(x)^* F(x), x \in H, \tag{4.17}$$

where $F'(x)^*$ denotes the Hilbert space adjoint of $F'(x), x \in H$.

Note that (4.17) is a universal form for gradients of functions ϕ given by (4.16).

Note that if $\Omega \subset H$ so that $F'(x)^*$ is uniformly bounded below for $x \in \Omega$, i.e., there is $d > 0$ so that $\|F'(x)^* g\|_H \geq d\|g\|_K, x \ \in \Omega,\ g \in K$, then ϕ satisfies (4.10) with $c = 2^{-1/2}d$. One can do better with the following:

Theorem 4.12. *Suppose there exist $M, b > 0$ so that if $g \in K$ and $x \in \Omega$, then for some $h \in H, \|h\|_H \leq M$,*

$$\langle F'(x)h, g\rangle_K \geq b\|g\|_K.$$

Then (4.7) holds with $c = \frac{2^{-1/2}b}{M}$.

Proof. Suppose $x \in \Omega$. Then

$$\begin{aligned}\|(\nabla\phi)(x)\|_H &= \sup_{h\in H, \|h\|_H = M} \frac{\langle h, F'(x)^* F(x)\rangle_H}{M} \\ &= \sup_{h\in H, \|h\|_H = M} \frac{\langle F'(x)h, F(x)\rangle_K}{M} \geq \frac{b}{M}\|F(x)\|_K\end{aligned}$$

since by hypothesis there is $h \in H$ such that $\|h\|_H \leq M$ and $\langle F'(x)h, F(x)\rangle_K \geq\ b\|F(x)\|_K$. □

Applications of Theorem 4.12 may be as follows: Many systems of nonlinear differential equations may be written (for appropriate H and K) as the problem of finding $u \in H$ such that $F(u) = 0$. The problem of finding h given $g \in K$, $u \in H$, such that

$$F'(u)h = g$$

then becomes a systems of linear differential equations. An abundant literature exists concerning existence of (and estimates for) solutions of such equations (cf [83, 219]). Thus linear theory holds the hope of providing gradient inequalities in specific cases.

As an application of Theorem 4.5 there is the following implicit function theorem due to A. Castro and this writer [37]. Compare results of Chapter 9.

Theorem 4.13. *Suppose that each of* H *and* K *is a Hilbert space,* $r, Q > 0, G$ *is a* $C^{(1)}$ *function from* H *to* K *which has a locally lipschitzian derivative and* $G(0) = 0$*. Suppose also that there is* $c_0 > 0$ *so that if* $u \in H, \|u\|_H \leq r$*, and* $g \in K, \|g\|_K = 1$*, then*

$$\langle G'(u)v, g\rangle_K \geq c_0 \text{ for some } v \in H \text{ with } \|v\|_H \leq Q. \tag{4.18}$$

If $y \in K$ *and* $\|y\|_K < rc_0/Q$ *then*

$$u = \lim_{t\to\infty} z(t) \text{ exists and satisfies } G(u) = y \text{ and } \|u\|_H \leq r$$

where z *is the unique function from* $[0, \infty)$ *to* H *so that*

$$z(0) = 0, z'(t) = -(G'(z(t)))^*(G(z(t)) - y),\ t \geq 0. \tag{4.19}$$

Proof. Define $c = c_0/Q$. Pick $y \in K$ such that $\|y\|_K < rc$ and define $F : H \to K$ by

$$F(x) = G(x) - y, x \in H.$$

Then $\|F(0)\|_K = \|y\|_K < rc$. Noting that $F' = G'$, by Theorem 4.5, for z satisfying (4.19),

$$u = \lim_{t\to\infty} z(t) \text{ exist and } F(u) = 0, i.e., G(u) = y.$$

By the argument for Theorem 4.5 it is clear that $\|u\|_H \leq r$. □

4.3 Work of Chill and Huang on Gradient Inequalities

I didn't know, for a number of years, that Łojasiewicz, [113], had shown that inequalities such as (4.10) hold in the neighborhood of a zero of a real analytic function on a finite dimensional space. Such inequalities are called Łojasiewicz inequalities. Łojasiewicz' result does not generalize directly to infinite dimensions. To see this, define $\phi(x) = \frac{1}{2}\|Tx\|^2$ for T a compact symmetric linear transformation from an infinite dimensional Hilbert space to itself. The Łojasiewicz result has been applied, however, in an infinite dimensional setting to determine convergence at infinity of solutions to some time dependent partial differential equations (cf [215]).

Works of Chill and coauthors, [39–43], and Huang, [85], contain a great deal of information on gradient inequalities. These works concern, for the most part, asymptotic convergence to a steady state solution for time-dependent partial differential equations, but also contain results that are more relevant to the present setting. In [39] there is a proof of a very general version of a Łojasiewic-Simon inequality. There is also a discussion of such results in [85]. This is a generalization of the classic Łojasiewic inequality to infinite dimensions under a restriction on the range of the transformation involved. This assumption is known to be satisfied in a number of substantial applications. In [43] there is special attention to Łojasiewic inequalities in Hilbert space. The works cited in this paragraph are related to the presentation in the present volume; a reader is encouraged to study these references in their original form and also to consult references cited in these works.

4.4 Higher Order Sobolev Spaces for Lower Order Problems

Sometimes it is useful to carry out steepest descent in a Sobolev space of higher order than absolutely required for formulation of a given problem. What follows is an indication of how that might come about. This work is taken from [164].

Suppose m is a positive integer, Ω is a bounded open subset of R^m and ϕ is a $C^{(1)}$ function from $H^{1,2}(\Omega)$ to $[0,\infty)$ which has a locally lipschitzian derivative. For each positive integer k denote the Sobolev space $H^{k,2}(\Omega)$ by H_k. Assume that Ω satisfies the cone condition (see [2] for this term as well as other matters concerning Sobolev spaces) in order to have that H_k is compactly embedded in $C_B^{(1)}(\Omega)$ for $2k > m+2$.

If k is a positive integer then denote by $\nabla_k\phi$ the function on H_1 so that

$$\phi'(y)h = \langle h, (\nabla_k\phi)(y)\rangle_{H_k},\ y \in H_1, h \in H_k. \tag{4.20}$$

This can be done since for each $y \in H_1$, the linear functional $\phi'(y)$ is a continuous linear functional on H_1 and hence its restriction to H_k is also a continuous linear functional on H_k. Each of the functions, $\nabla_k\phi, k = 1, 2, \ldots$ is called a Sobolev gradient of ϕ.

Lemma 4.14. *If k is a positive integer then $\nabla_k\phi$ is locally lipschitzian on H_k as a function from H_1 to H_k.*

Proof. Suppose $w \in H_k$. Denote by each of r and L a positive number so that if $x, y \in H_1$ and $\|x-w\|_{H_1}, \|y-w\|_{H_1} \le r$, then

$$\|(\nabla_1\phi)(x) - (\nabla_1\phi)(y)\|_{H_1} \le L\|x-y\|_{H_1}. \tag{4.21}$$

Now suppose that $x, y \in H_1$ and

$$\|x - w\|_{H_1}, \|y - w\|_{H_1} \leq r.$$

Then

$$\begin{aligned}
\|(\nabla_k \phi)(x) - (\nabla_k \phi)(y)\|_{H_k} &= \sup_{h \in H_k, \|h\|_{H_k}=1} \langle (\nabla_k \phi)(x) - (\nabla_k \phi)(y), h \rangle_{H_k} \\
&= \sup_{h \in H_k, \|h\|_{H_k}=1} (\phi'(x)h - \phi'(y)h) \\
&= \sup_{h \in H_k, \|h\|_{H_k}=1} \langle (\nabla_1 \phi)(x) - (\nabla_1 \phi)(y), h \rangle_{H_1} \\
&\leq \sup_{h \in H_k, \|h\|_{H_k}=1} \|h\|_{H_1} \|\nabla_1 \phi)(x) - (\nabla_1 \phi)(y)\|_{H_1} \\
&\leq \sup_{h \in H_k, \|h\|_{H_k}=1} \|h\|_{H_k} \|\nabla_1 \phi)(x) - (\nabla_1 \phi)(y)\|_{H_1} \\
&\leq L\|x - y\|_{H_1}.
\end{aligned}$$

□

In particular, $\nabla_k \phi$ is continuous as a function from H_1 to H_k.

Theorem 4.15. *In addition to the above assumptions about ϕ, suppose that*

$$\phi'(y)y \geq 0, \ y \in H_1. \tag{4.22}$$

If k is a positive integer, $x \in H_k$ and

$$z(0) = x, z'(t) = -(\nabla_k \phi)(z(t)), \ t \geq 0, \tag{4.23}$$

then $R(z)$, the range of z, is a subset H_k and is bounded in H_k.

Proof. First note that one has, using Theorem 4.1, existence and uniqueness for (4.23) since the restriction of $\nabla_k \phi$ is locally lipschitzian as a function from H_k to H_k and ϕ is bounded below. Since $x \in H_k$, for z as in (4.23), it must be that $R(z) \subset H_k$ and

$$\begin{aligned}
(\|z\|_{H_k}^2/2)'(t) &= \langle z'(t), z(t) \rangle_{H_k} \\
&= -\langle (\nabla_k \phi)(z(t)), z(t) \rangle_{H_k} = -\phi'(z(t))z(t) \leq 0, \ t \geq 0.
\end{aligned}$$

Thus $\|z\|_{H_k}^2$ is nonincreasing and so $R(z)$ is bounded in H_k. □

Assume for the remainder of this section that $2k > m + 2$. Observe that for z as in Theorem 4.15, $R(z)$ is precompact in $C_B^{(1)}$ and hence also in H_1. For $x \in H_k$ and z satisfying (4.23) denote by Q_x the H_1 $\omega-$ limit set of z, i.e.,

$$Q_x = \{y \in H_1 : y = H_1 - \lim_{n \to \infty} z(t_n), \{t_n\}_{n=1}^{\infty} \text{ increasing, unbounded}\}.$$

Theorem 4.16. *If* $x \in H_k$ *and* $y \in Q_x$, *then* $(\nabla_k \phi)(y) = 0$.

Proof. Note that

$$(\phi(z))'(t) = \phi'(z(t))z'(t) = -\|(\nabla_k \phi)(z(t))\|^2_{H_k}$$

and so

$$\phi(z(0)) - \phi(z(t)) = \int_0^t \|(\nabla_k \phi)(z)\|^2_{H_k}$$

and hence

$$\int_0^\infty \|(\nabla_k \phi)(z)\|^2_{H_k} < \infty. \tag{4.24}$$

Thus if

$$u = H_1 - \lim_{t \to \infty} z(t)$$

exists, then by (4.24), $(\nabla_k \phi)(u) = 0$ since, by Lemma 4.14, $\nabla_k \phi$ is continuous as a function from H_1 to H_k and z is continuous as a function from $[0, \infty)$ to H_1. Thus the conclusion holds in this case.

Suppose now that

$$H_1 - \lim_{t \to \infty} z(t) \text{ does not exist}$$

and that $y \in Q_x$ but $(\nabla_k \phi)(y) \neq 0$. Then $(\nabla_1 \phi)(y) \neq 0$ also. Denote by each of α, M a positive number so that

$$\|(\nabla_k \phi)(x)\|_{H_1} \geq M$$

if $\|x - y\|_{H_1} \leq \alpha$. Then there are increasing sequences $\{a_i\}_{i=1}^\infty, \{b_i\}_{i=1}^\infty$ so that

$$\begin{aligned} H_1 - \lim_{n \to \infty} z(a_n) &= y, \\ \|z(b_n) - y\| &= \alpha, \\ \|z(a_n) - z(b_n)\| &\geq \alpha/2, \\ \text{and } \|z(t) - y\| &\leq \alpha, n = 1, 2, \ldots, \end{aligned}$$

and so

$$\begin{aligned} (\alpha/2)^2 &\leq \|z(b_i) - z(a_i)\|^2_{H_1} = \|\int_{a_i}^{b_i} z'\|^2_{H_1} \\ &\leq (\int_{a_i}^{b_i} \|z'\|_{H_1})^2 \leq (b_i - a_i)(\int_{a_i}^{b_i} \|z'\|^2_{H_1}) \leq (b_i - a_i)(\int_{a_i}^{b_i} \|z'\|^2_{H_k}). \end{aligned}$$

Hence

$$b_i - a_i \geq (\alpha/2)^2 / (\int_{a_i}^{b_i} \|z'\|^2_{H_k})$$

and so $\lim_{i\to\infty}(b_i - a_i) = \infty$ due to (4.24). But

$$\|(\nabla_k \phi)(z(t))\|_{H_1} \geq M,\ t \in [a_i, b_i],\ i = 1, 2, \ldots$$

and thus

$$\infty > \int_0^\infty \|z'\|_{H_1}^2 \geq \sum_{i=1}^\infty \int_{a_i}^{b_i} \|z'\|_{H_1}^2 = \infty,$$

a contradiction. Thus $(\nabla_k \phi)(y) = 0$. □

Condition (4.22) is perhaps too strong to apply to many systems of partial differential equations. Note however, that this condition does not imply convexity. It is hoped that Theorem 4.15 will lead to results in which (4.22) is weakened while still allowing the above conclusions.

Chapter 5
Orthogonal Projections, Adjoints and Laplacians

This chapter contains background that underlies the theory of Sobolev gradients. In particular there is a discussion of adjoints, as in (4.17), and how they relate to the orthogonal projections which are at the center of the theory.

Suppose H, K are Hilbert spaces and $T \in L(H, K)$, the space of all bounded linear transformations from H to K. It is customary to denote by T^* the member of $L(K, H)$ so that

$$\langle Tx, y\rangle_K = \langle x, T^*y\rangle_H,\ x \in H,\ y \in K. \tag{5.1}$$

In applications to differential equations, H is often taken to be a Sobolev space (which is also a Hilbert space) and K to be an L_2 space. In order to illustrate how gradient calculations depend upon adjoint calculations, first examine the simplest setting for a Sobolev space. Our general reference for linear transformations on Hilbert spaces is [204].

In [225], Weyl deals with the problem of determining when a vector field is the gradient of some function. He introduces certain orthogonal projections to solve this problem for all square integrable (but not necessarily differentiable) vector fields. Our construction of Sobolev gradients is related to work of Weyl [225], von Neumann [223], Beurling and Deny [21, 22].

5.1 A Construction of a Sobolev Space

A construction of a simple Sobolev space is given here in order to make our exposition more nearly self contained. Consult [2] for extensive background on Sobolev spaces.

Take $K = L_2([0, 1])$ and define $H = H^{1,2}([0, 1])$ to be the set of all first terms of members of $cl(Q)$, where

$$Q = \{\tbinom{u}{u'} :\ u \in C^1([0, 1])\} \tag{5.2}$$

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_5,

and the closure $cl(Q)$ is taken in $K \times K$. The following is a crucial fact which has its counterpart in construction of probably all Sobolev spaces:

Lemma 5.1. *$cl(Q)$ is a function in the sense that no two members of $cl(Q)$ have the same first term.*

Proof. Suppose that $\binom{f}{g}, \binom{f}{h} \in cl(Q)$ and $k = g - h$. Then $\binom{0}{k} \in cl(Q)$. Denote by $\{\binom{f_n}{f_n'}\}_{n=1}^{\infty}$ a sequence in Q which converges to $\binom{0}{k}$. If $m, n \in Z^+$, denote by $c_{m,n}$ a member of $[0,1]$ so that

$$|(f_m - f_n)(c_{m,n})| \leq |(f_m - f_n)(t)|,\ t \in [0,1].$$

Then if $t \in [0,1]$,

$$f_m(t) - f_n(t) = f_m(c_{m,n}) - f_n(c_{m,n}) + \int_{c_{m,n}}^{t} (f_m' - f_n')$$

and so

$$\begin{aligned} |(f_m(t) - f_n(t)| &\leq \|f_m - f_n\|_K + |\int_{c_{m,n}}^{t} (f_m' - f_n')| \\ &\leq \|f_m - f_n\|_K + (\int_{c_{m,n}}^{t} (f_m' - f_n')^2)^{1/2} \\ &\leq \|f_m - f_n\|_K + (\int_0^1 (f_m' - f_n')^2)^{1/2} \to 0 \text{ as } m, n \to 0. \end{aligned}$$

Hence $\{f_n\}_{n=1}^{\infty}$ converges uniformly to 0 on [0,1] since it already converges to 0 in K. Note that if $t, c \in [0,1]$,

$$(\int_c^t f_n' - \int_c^t k)^2 \leq (\int_c^t |f_n' - k|)^2 \leq \int_c^t (f_n' - k)^2 \leq \|f_n' - k\|_K^2 \to 0 \text{ as } n \to \infty,$$

and so

$$\lim_{n\to\infty} \int_c^t f_n' = \int_c^t k.$$

Therefore since

$$f_n(t) - f_n(c) = \int_c^t f_n',$$

it follows that

$$0 = \int_c^t k,\ c, t\ \in [0,1].$$

But this implies that $k = 0$ and hence $g = h$. □

If $\binom{f}{g} \in cl(Q)$, then, by definition, $f' = g$. Also define

$$\|f\|_H = (\|f\|_K^2 + \|f'\|_K^2)^{1/2}.$$

If $f \in C^1$ then this definition is consistent with the usual definition. In fact, if $g \in K$, $c \in R$ and

$$f(t) = c + \int_0^t g,\ t \in [0,1],$$

then $f \in H$ and $\binom{f}{g} \in Q$ and so in the above sense, $f' = g$. Moreover, every member of H arises in this way.

To illustrate a point of view on adjoints of linear differential operators, consider the member T of $L(H, K)$ defined simply by

$$Tf = f',\ f \in H.$$

Problem. Find a construction for T^* as a member of $L(H, K)$.

Solution. First identify a subset of $Q^\perp$ as

$$L = \{\binom{v'}{v} \mid v \in C^1([0,1]),\ v(0) = 0 = v(1)\}.$$

It is an elementary problem in ordinary differential equations to deduce that if $f, g \in C([0,1])$, then there are unique $\binom{u}{u'} \in Q$ and $\binom{v'}{v} \in S$ so that

$$\binom{u}{u'} + \binom{v'}{v} = \binom{f}{g}.$$

Explicitly, using

$$C(t) = \cosh(t), S(t) = \sinh(t),\ t \in R, \tag{5.3}$$

we have

$$u(t) = [C(1-t)\int_0^t (C(s)f(s) + S(s)g(s))\ ds$$
$$+ C(t)\int_t^1 (C(1-s)f(s) - S(1-s)g(s))\ ds]/S(1),\ t \in [0,1],$$
$$v(t) = [S(1-t)\int_0^t (C(s)f(s) + S(s)g(s))\ ds$$
$$- S(t)\int_t^1 (C(1-s)f(s) - S(1-s)g(s))\ ds]/S(1),\ t \in [0,1].$$

Observe that L and Q are mutually orthogonal and their direct sum is dense in $K \times K$. Therefore $K \times K$ is the direct sum of the closures of Q and L. Since (5.3) may be extended by continuity to any $\binom{f}{g} \in K \times K$, it follows that

$$P\binom{f}{g} = \binom{u}{u'} \tag{5.4}$$

where u is given by (5.3), and it is only assumed that $f, g \in L_2([0,1])$. This leads to an explicit expression P.

To finish the solution, suppose that $f \in H$ and $g \in K$. Then

$$\langle Tf, g\rangle_K = \langle f', g\rangle_K = \langle \binom{f}{f'}, \binom{0}{g}\rangle_{K\times K} = \langle \binom{f}{f'}, P\binom{0}{g}\rangle_{K\times K} = \langle f, \pi P\binom{0}{g}\rangle_H$$

where $\pi\binom{r}{s} = r$ if $r, s \in K$. Hence

$$T^*g = \pi P\binom{0}{g}.$$

Since P is explicitly given, so is T^*.

The next section gives a more general account on how a single transformation T can have two very different, but related, adjoints.

5.2 A Formula of von Neumann

Adjoints as just calculated have a close relation with the adjoints of unbounded closed linear transformations. Recall the following from [204, 223], for example: If W is a closed linear transformation on a dense linear subset of H to K, i.e.,

$$\{\binom{x}{Wx} \ : \ x \in D(W)\}$$

is a closed subspace of $H \times K$, then an adjoint W^t of W is defined by:

$$D(W^t) = \{y \in K : \exists z \in H \text{ such that } \langle Wx, y\rangle_K = \langle x, z\rangle_H,\ x \in D(W)\},$$
$$W^t y = z, \quad \text{with } y, z \text{ as above.}$$

From this definition it follows that if $x \in D(W)$, $y \in D(W^t)$, then

$$\langle \binom{x}{Wx}, \binom{-W^t y}{y}\rangle_{H\times K} = \langle Wx, y\rangle_K - \langle x, W^t y\rangle_H = 0. \tag{5.5}$$

Furthermore, it is an easy consequence of the definition that

$$\{\binom{x}{Wx} \ : \ x \in D(W)\}^{\perp} = \{\binom{-W^t y}{y} \ : \ y \in D(W^t)\}$$

and consequently that if $\binom{r}{s} \in H \times K$, then there exists uniquely $x \in D(W)$, $y \in D(W^t)$ such that

$$\binom{x}{Wx} + \binom{-W^t y}{y} = \binom{r}{s}. \tag{5.6}$$

The following is from [223] and is due to von Neumann::

Theorem 5.2. *Suppose W is a closed, densely defined linear transformation on the Hilbert space H to the Hilbert space K. Then the orthogonal projection of $H \times K$ onto*

$$\{\left(\begin{smallmatrix} x \\ Wx \end{smallmatrix}\right) \,:\, x \in D(W)\} \tag{5.7}$$

is given by the 2×2 *matrix:*

$$\begin{pmatrix} (I + W^tW)^{-1} & W^t(I + WW^t)^{-1} \\ (I + W^tW)^{-1} & I - (I + WW^t)^{-1} \end{pmatrix}. \tag{5.8}$$

Proof. Note first that if r, s are as in (5.6) and $s = 0$, then $x - W^t y = r$, $Wx + y = 0$ and consequently

$$(I + W^tW)y = r.$$

Hence the range of $(I + W^tW) = H$. Since if $x \in D(W^tW)$,

$$\langle (I + W^tW)x, x\rangle_H \geq \langle x, x\rangle_H$$

it follows that

$$(I + W^tW)^{-1} \in L(H, H), \text{ and } |(I + W^tW)^{-1}| \leq 1.$$

Similar properties hold for $(I+WW^t)^{-1}$. It is easily checked that the matrix indicated (5.8) is idempotent, symmetric, fixed on the set (5.11) and has range that set since

$$W(I + W^tW)^{-1}x = (I + WW^t)^{-1}Wx,\ x \in D(W)$$

and

$$W^t(I + WW^t)^{-1}y = (I + W^tW)^{-1}W^t y,\ y \in D(W^t)).$$

Hence the matrix (5.8) is the orthogonal projection onto the set in (5.7). □

5.3 Relationship Between Adjoints

To see a relationship between the adjoints W^t, W^* of the above two sections, take W to be the closed densely defined linear transformation on K defined by $Wf = f'$ for exactly those members of K which are also members of $H^{1,2}([0, 1])$. Then the projection P in Section 5.1 is just the orthogonal projection onto the set in (5.11) which in this case is the same as $cl(Q)$. See [56] for an additional description of adjoints of linear differential operators when they are considered as densely defined closed operators.

More generally this relationship may be summarized by the following:

Theorem 5.3. *Suppose that each of H and K is a Hilbert space, W is a closed densely defined linear transformation of H to K. Suppose in addition that J is the Hilbert space whose points consist of $D(W)$ with*

$$\|x\|_J = (\|x\|_H^2 + \|Wx\|_K^2)^{1/2},\ x \in J. \tag{5.9}$$

Then the adjoint W^* of W **(with W regarded as a member of $L(J,K)$)** *is given by*

$$W^*y = \pi P\binom{0}{y},\ y \in J,$$

where P is the orthogonal projection of $H \times K$ onto $\{\binom{x}{Wx} : x \in J\}$ and $\pi\binom{r}{s} = r,\ \binom{r}{s} \in H \times K$.

Proof. If $x \in D(W)$,

$$\begin{aligned}\langle Wx, y\rangle_K &= \langle \tbinom{x}{Wx}, \tbinom{0}{y}\rangle_{H\times K} = \langle \tbinom{x}{Wx}, P\tbinom{0}{y}\rangle_{H\times K} \\ &= \langle x, \pi P\tbinom{0}{y}\rangle_J, \text{ so that } W^*y = \pi P\tbinom{0}{y}.\end{aligned}$$

□

It is emphasized that W has two separate adjoints: one regarding W as a closed densely defined linear transformation on H to H and the other regarding W as a bounded linear transformation on $D(W)$ where the norm on $D(W)$ is the graph norm (5.9). We will try to use the separate symbols W^t, W^* for these two distinct (but related objects). At any rate, it is an obligation of a writer to make clear in a given context which adjoint is being discussed. In Chapter 8 there is a one parameter family of adjoints of a given linear transformation, even in a finite dimensional setting. In Chapter 15 this occurs again in a study of Tricomi's equation.

5.4 General Laplacians

Suppose that H is a Hilbert space and H' is a dense linear subspace of H which is also a Hilbert space under the norm $\|\ \|_{H'}$ in such a way that

$$\|x\|_H \le \|x\|_{H'},\ x \in H'.$$

Following Beurling-Deny [21, 22], for the pair (H, H') there is an associated transformation called the laplacian for (H, H'). It is described as follows. Pick $y \in H$ and denote by f the functional on H corresponding to y :

$$f(x) = \langle x, y\rangle_H,\ x \in H.$$

Denote by k the restriction of f to H'. Then

$$|k(x)| = |\langle x, y\rangle_H| \le \|x\|_H \|y\|_H \le \|x\|_{H'} \|y\|_H,\ x \in H'.$$

Hence k is a continuous linear functional on H' and so there is a unique member z of H' such that

$$k(x) = \langle x, z\rangle_{H'},\ x \in H'.$$

Define $M : H \to H'$ by $My = z$ where y, z are as above. It will be seen that M^{-1} exists; it will be called the laplacian for the pair (H, H'). If H'_0 is a closed subspace of H' whose points are also dense in H, the corresponding transformation will be denoted by M_0.

The following is from [97].

Theorem 5.4. *M as defined above has the following properties:*

1. *$R(M)$ is dense in H*
2. *M^{-1}exists*
3. *$|M|_{L(X,Y)} \le 1$ where $X = H, H'$ and $Y = H, H'$*
4. *$\langle x, My\rangle_H = \langle Mx, y\rangle_H \forall x, y \in H$*
5. *$\langle x, My\rangle_{H'} = \langle Mx, y\rangle_{H'} \forall x, y \in H'$*
6. *M as a transformation from H to H has a square root, $\sqrt{M}$, M from H' to H' has a square root, $\sqrt{M_{H'}}$, and $\sqrt{M}$ agrees with $\sqrt{M_{H'}}$ on H'.*
7. *If $x \in H'$, then $\|x\|_H = \|\sqrt{M}x\|_{H'}$.*
8. *If $x \in H$, then $\|x\|_H = \|\sqrt{M}x\|_{H'}$.*
9. *The range of $\sqrt{M}$ is H'.*

Note that 9) gives a very general solution to the symmetric case of Kato's square root problem (see for example [5]).

Proof. Suppose first that there is $z \in H'$ so that $\langle z, Mx\rangle_{H'} = 0, x \in H$. Then

$$0 = \langle z, Mz\rangle_{H'} = \langle z, z\rangle_H$$

and so $z = 0$. Thus $cl_{H'} R(M) = H'$. But then

$$H' = cl_{H'}(R(M)) \subset cl_H(R(M)).$$

Hence

$$H = cl_H(H') = cl_H(R(M))$$

and (a) is demonstrated. To show that 2) holds, suppose that $x \in H$ and $Mx = 0$. Then

$$0 = \langle z, Mx\rangle_{H'} = \langle z, x\rangle_H,\ z \in H'.$$

But this implies that $z = 0$ since the points of H' are dense in H.

To show 3), note that for $x \in H$

$$\begin{aligned}\|Mx\|_H \le \|Mx\|_{H'} &= \sup\{\langle z, Mx\rangle_{H'} : \|z\|_{H'} = 1\} \\ &= \sup\{\langle z, x\rangle_H : \|z\|_{H'} = 1\} \le \|x\|_H \le \|x\|_{H'}\end{aligned}$$

The second to last inequality is due to the Cauchy-Schwarz inequality.

To show 4) let $x, y \in H$. Then

$$\langle Mx, y\rangle_H = \langle Mx, My\rangle_{H'} = \langle x, My\rangle_H.$$

To show 5), let $x, y \in H'$. Then

$$\langle Mx, y\rangle_{H'} = \langle x, y\rangle_H = \langle x, My\rangle_{H'}.$$

To show 6), use from [204] the fact that a positive, symmetric bounded linear transformation from a Hilbert space to itself has a unique positive, symmetric bounded square root (which also commutes with the given transformation). $M : H' \to H'$ is symmetric by 5) and bounded by 3). $M : H' \to H'$ is also positive definite because for $x \in H'$ $\langle Mx, x\rangle_{H'} = \|x\|_H^2$.

Denote the positive square root of M, as a transformation from H' to H', by $\sqrt{M}_{H'}$. Hence for $x \in H'$,

$$\|x\|_H^2 = \langle x, Mx\rangle_{H'} = \langle \sqrt{M}_{H'}x, \sqrt{M}_{H'}x\rangle_{H'} = \|\sqrt{M}_{H'}x\|_{H'}^2$$

and 7) is done.

Note that M as a transformation from H to H is also positive since $\langle Mx, x\rangle_H = \langle Mx, Mx\rangle_{H'}$. It is also bounded and symmetric by parts 3) and 4). Hence M as a transformation from H to H has a positive square root. Call this square root $\sqrt{M}$.

With M regarded as a member of $L(H)$, note that (see [204]) the sequence $\{Y_n\}_{n=0}^{\infty}$ defined by

$$Y_0 = 0,\ Y_{n+1} = (I - M) + \frac{1}{2}Y_n^2,\ n = 0, 1, \ldots$$

converges in H to $\sqrt{M}$. Now with $M_{H'}$, the restriction of M to H', this sequence (or rather the terms of this sequence restricted to H') converges to $\sqrt{M_{H'}}$ where each member is now regarded as a member of $L(H')$. One can then observe that 6) holds.

To show 8) suppose $x \in H$. Then there exists a sequence of points, $x_1, x_2, \ldots$ belonging to H' so that the $H - \lim_n x_n = x$. For each n, $\|x_n\|_H = \|\sqrt{M}x_n\|_{H'}$. Since $\{x_n\}_{n\ge1}$ is Cauchy in H, it converges in H and hence $\{\sqrt{M}x_n\}_{n\ge1}$ converges in H'. Call this limit z_x. It will be shown that $z_x = \sqrt{M}x$. Note that

$$\|z_x - \sqrt{M}x\|_H \le \|z_x - \sqrt{M}x_n\|_H + \|\sqrt{M}x_n - \sqrt{M}x\|_H.$$

Given ϵ there is n so that the right side of this equation is less than ϵ since

- $H' - \lim_n \sqrt{M}x_n = z_x$ implies $H - \lim_n \sqrt{M}x_n = z_x$.
- $\sqrt{M}$ is continuous from H to H.

Hence for $x \in H$, $\sqrt{M}x = z_x$. This also shows that $R(\sqrt{M}) \subseteq H'$. So now for $x \in H$, let x_n be a sequence in H' converging to x in H. Then

$$\|x\|_H = \lim_{n\to\infty} \|x_n\|_H = \lim_{n\to\infty} \|\sqrt{M}x_n\|_{H'} = \|\sqrt{M}x\|_{H'}$$

and 8) is done.

Finally to show $R(\sqrt{M}) = H'$, note that in the proof of 8) it held that $R(\sqrt{M}) \subseteq H'$. Finish 9) by showing that the range of $\sqrt{M}$ is dense and closed in H'. To show $\sqrt{M}$ is closed, suppose $\{\sqrt{M}x_n\}_{n\geq 1}$ converges in H' to y. Then

$$\|\sqrt{M}x_n\|_{H'} = \|x_n\|_H, \{x_n\}_{n\geq 1},$$

is Cauchy in H. Let x be the H limit of $\{x_n\}_{n=1}^{\infty}$. Then $\sqrt{M}x = y$ since

$$\|\sqrt{M}x - y\|_H \leq \|\sqrt{M}x - \sqrt{M}x_n\|_H + \|\sqrt{M}x_n - y\|_H \text{ and}$$

given $\epsilon > 0$, there exists an n so that the right side of the inequality is less than ϵ. Hence $\sqrt{M}x = y$.

Now show $\sqrt{M}$ is injective. By 2) M is injective. So if

$$\sqrt{M}x = 0, \text{ then } Mx = \sqrt{M}\sqrt{M}x = 0 \text{ and so } x = 0.$$

To show the range of $\sqrt{M}$ is dense in H', suppose there exists $y \in H'$ so that

$$\langle \sqrt{M}x, y\rangle_{H'} = 0 \text{ for all } x \in H.$$

Then if $x = \sqrt{M}y$,

$$\langle \sqrt{M}\sqrt{M}y, y\rangle_{H'} = \langle \sqrt{M}y, \sqrt{M}y\rangle_{H'} = \|\sqrt{M}y\|_{H'} = 0.$$

This implies that $\sqrt{M}y = 0$ so $y = 0$. Thus the range of $\sqrt{M}$ is a dense and closed subspace of H' so it is equal to H'. □

Since M is a symmetric member of $L(H,H)$, there is a spectral representation α of M in the form

$$M = \int_0^1 j d\,\alpha \tag{5.10}$$

where j is the identity transformation on $[0,1]$ and α is the appropriate resolution of the identity (see [204]), first noting that $[0,1]$ contains the numerical range of M. It follows that since M is positive definite, then for each $\lambda \geq 0$, there is a unique positive definite symmetric fractional power M^λ and that if $T : [0,\infty) \to L(H,H)$ is defined by $T(\lambda) = M^\lambda,\ \lambda \geq 0$, then we have

Theorem 5.5. *T is a strongly continuous one parameter semigroup of linear transformations on H in the sense that*

$$T(0) = I,\ T(t)T(s) = T(t+s),\ t, s \geq 0 \tag{5.11}$$

and, if $x \in H$, then

$$\lim_{t \to 0+} T(t)x = x. \tag{5.12}$$

Proof. Part (5.11) follows directly from the spectral theorem (cf. [204]). To show (5.12), note that also from the spectral theorem, if $x \in H, t \geq 0$, then

$$x - M^t x = \int_0^1 (1 - j^t) d\ \alpha x. \tag{5.13}$$

(α as in (5.10)). Note that the functions

$$1 - j^t,\ t \geq 0,$$

converge pointwise nondecreasing, as $t \to 0+$, to the step function on $[0, 1]$ which is zero on $(0, 1]$ and is one at 0. Thus from (5.13), $x - M^t x$ converges, as $t \to \infty$, to the orthogonal projection of x onto $N(M)$. But $N(M) = \{0\}$ and hence

$$\lim_{t \to 0} T(t)x = x.$$

□

For each $s > 0$, define H_s to be the Hilbert space whose points are $R(M^{s/2})$ and

$$\|x\|_{H_s} = \|M^{-s/2}x\|_H,\ x \in H_s. \tag{5.14}$$

Actually, this definition makes sense for all $s \in R$ with H_{-1}, for example, having the norm

$$\|x\|_{H_{-1}} = \|M^{1/2}x\|_H,\ x \in R(M^{-1/2}).$$

Theorem 5.6. *$H' = H_1$.*

Proof. By item 9 of Theorem 5.4, the points of H_1 and H' are the same. If $x \in H_1$, then

$$\begin{aligned}\|x\|_{H_1}^2 &= \|M^{-1/2}x\|_H^2 = \langle M^{-1/2}x, M^{-1/2}x\rangle_H \\ &= \langle M^{-1/2}x, MM^{-1/2}x\rangle_{H'} = \langle x, x\rangle_{H'} = \|x\|_{H'}^2,\end{aligned}$$

so that H_1 and H' are the same Hilbert space. □

The spaces $H_{m/2},\ m \geq 0$, can be a basic for dealing with fractional power Sobolev spaces of the type $H^{m,2}(\Omega)$, where Ω is a region in a finite dimensional Euclidean space.

5.5 Extension of Projections Beyond Hilbert Spaces

This section describes some recent work of P. Kazemi, [98], which extends some of the projections of the previous section to some non-Hilbert spaces. In Chapter 14 it will be seen how this is used to prove convergence of steepest descent for some Ginzburg-Landau functionals of superconductivity. Work in [98] deals with the following setting: Choose $2 \le n \le 4$. Denote by Ω a bounded open region in R^n that satisfies the cone condition (see [2]). Let $K = L_2(\Omega),\ H = H^{1,2}(\Omega)$ and write L_p for $L_p(\Omega)$. Define

$$W = \{\begin{pmatrix} u \\ \nabla u \end{pmatrix} : u \in H\}.$$

Pick p, q so that $p \in (1,2),\ p = \frac{q}{1-q}$, H is embedded in $L_q(\Omega)$ and, if $f, g \in H$, then $fh \in L_p$ where h is any partial derivative of g. Define

$$S_p = \{f = (f(0), f(1), \dots, f(n))\}$$

with

$$\|f\|_{S_p} = \|f(0)\|_{L_p} + \sum_{i=1}^{n} \|f(i)\|_K.$$

If $f \in L_p,$ and $u \in H$, use the notation

$$\langle f, u\rangle_K \text{ to mean } \int_\Omega fu,$$

and define, for $f \in S_p, u \in H$,

$$\langle f, u\rangle_K^{n+1} \text{ to mean } \int_\Omega f(0)u + \sum_{i=1}^{n} \int_\Omega f(i)u_i,$$

where u_i is the partial derivative of u in the $i-th$ coordinate direction. Use $u \in W$ to mean that $u = \binom{w}{\nabla w}$ for some $w \in H$ (after all, W *is* a collection of ordered pairs). Following [98], for $f \in S_p$, define

$$\alpha_f(u) = \langle u, f\rangle_{K^{n+1}},\ u \in W.$$

It is then shown that there is $w \in H$ so that

$$\alpha_f(u) = \langle u, w\rangle_H,\ u \in H. \tag{5.15}$$

For $f \in S_p$, define $Pf = v$ where $v = \binom{w}{\nabla w}$ and w is as in (5.15).

Theorem 5.7. *With this definition:*

- $\langle Pg, f\rangle_{K^{n+1}} = \langle g, Pf\rangle_{K^{n+1}},\ g \in W.$
- $P(Pf) = Pf,\ f \in S_p.$
- $\|Pf\|_{K^{n+1}} \leq c\|f\|_{S_p},\ c = \max(c_1, 1),$

c_1 *being the embedding constant for the pair* L_q, H.

This result extends P to S_p. Call the extension P also.

Denote by M the transformation from K to H satisfying

$$\langle u, v\rangle_K = \langle u, Mv\rangle_H,\ u \in H$$

(see previous section). Extend M to $M_p : L_p \to H$ so that if $v \in L_p$, then

$$\langle u, v\rangle_K = \langle u, M_p v\rangle_H,\ u \in H.$$

Theorem 5.8. *With this definition:*

- M_p *is injective.*
- $M_p \in L(X, Y),\ X, Y = H, L_p.$
- *If* $\{f_k\}_{k=1}^{\infty}$, *is bounded in* L_p, *then* $\{M_p f_k\}_{k=1}^{\infty}$ *has a subsequence which converges in* K *to some* $v \in H$.

Theorem 5.9. *The* 2×2 *matrix* P *is defined by*

$$P = \begin{pmatrix} M_p & W^t(I + WW^t)^{-1} \\ WM_p & I - (I + WW^t)^{-1} \end{pmatrix},$$

with domain S_p.

Proofs of Theorems 5.7, 5.8, 5.5 are found in [98]. As mentioned, these will be used in Chapter 14. Results in this section are representative of a wide class of generalizations of the previous section and they are an important contribution to the theory of Sobolev gradients.

5.6 A Generalized Lax-Milgram Theorem

In this section there is an extension of the Lax-Milgram [105] Theorem. The work of this section is taken from [165]. Denote by each of H, H_0', H' a Hilbert space with

$$H_0' \subset H' \subset H$$

so that

$$\|x\|_{H_0'} = \|x\|_{H'}, x \in H_0'$$

and

$$\|x\|_H \le \|x\|_{H'}, x \in H'.$$

Suppose also that the points of H'_0, H' are dense in H. Define P_0 to be the orthogonal projection of H' onto H'_0 and denote the complementary projection $I - P_0$ by Q_0. For an example, one can take

$$H = L_2([0,1]), H' = H^{1,2}([0,1])$$

and

$$H'_0 = \{f \in H' : f(0) = 0 = f(1)\}.$$

Returning to the general case of H, H', H'_0, define

$$\beta(u) = (1/2)\|u\|^2_{H'} - \langle u, g\rangle_H,\ u \in H'. \tag{5.16}$$

Theorem 5.10. *Suppose $g \in H, w \in H'$ and $\beta : H' \to R$ is defined by (5.16). Then the minimum of $\beta(u)$ subject to the condition $Q_0 u = Q_0 w$ is achieved by*

$$u = Q_0 w + M_0 g. \tag{5.17}$$

The condition $Q_0 u = Q_0 w$ may be regarded as a generalized boundary or supplementary condition; it is equivalent to asking that the $u - w \in H'_0$.

Proof. Define $q = Q_0 w$ and define $\gamma : H'_0 \to R$ by

$$\gamma(y) = \beta(y + q),\ y \in H'_0.$$

Note that

$$\gamma'(y)k = \beta'(y + q)k = \langle y + q, k\rangle_{H'} - \langle k, g\rangle_H,\ k \in H'_0.$$

Note also that since

$$\gamma''(y)(k, k) = \|k\|^2_H,\ k, y \in H'_0,$$

it follows that γ is (strictly) convex. Now

$$\begin{aligned}\beta(u) &= (1/2)\|u\|^2_{H'} - \langle u, g\rangle_H \ge (1/2)\|u\|^2_{H'} - \|u\|_H\|g\|_H.\\ &\ge (1/2)\|u\|^2_{H'} - \|u\|_{H'}\|g\|_H = \|u\|_{H'}(\|u\|_{H'}/2 - \|g\|_H),\ u \in H'\end{aligned}$$

so β and hence γ is bounded from below.

Since γ is convex and bounded from below it has an absolute minimum if and only if it has a critical point. Moreover, such a critical point would be the unique point at which β attains its minimum. Observe that

$$\gamma'(y)k = \langle y + q, k\rangle_{H'} - \langle k, g\rangle_H = \langle y, k\rangle_{H'} - \langle k, g\rangle_H$$

since $\langle q, k\rangle_{H'} = 0,\ k \in H_0'$. Now

$$\langle k, g\rangle_H = \langle y, k\rangle_{H'},\ k \in H_0'$$

if and only if $y = M_0 g$. Choosing y in this way thus yields a critical point of γ. Consequently $u = y + q$ is the point of H' at which β attains its minimum. Therefore

$$u = Q_0 w + M_0 g$$

is the point at which β attains its minimum and the theorem is proved. □

5.7 Laplacians and Closed Linear Transformations

We now turn to a somewhat more concrete case of the above - a case which is closer to the example in Section 5.1.

Suppose that each of H and K is a Hilbert space and T is a closed and densely defined linear transformation on H to K. Let H' be the Hilbert space whose points are those of $D(T)$ where

$$\|x\|_{H'} = \|\tbinom{x}{Tx}\|_{H\times K},\ x \in D(T). \tag{5.18}$$

Suppose that the linear transformation T_0 is a closed, densely defined restriction of T (see [204] for a discussion of closed unbounded linear operators from one Hilbert space to another). Denote by H_0' the Hilbert space whose points are those of $D(T_0)$ where

$$\|x\|_{H_0'} = \|\tbinom{x}{T_0x}\|_{H\times K},\ x \in D(T_0). \tag{5.19}$$

Then H, H', H_0' fit the hypothesis of Theorem 5.10.

Here is an equivalent definition of T^t. The domain of T^t is

$$\{y \in H : x \to \langle Tx, y\rangle_K \text{ is continuous}\}.$$

For $y \in D(T^t), T^t y$ is the element of H such that

$$\langle Tx, y\rangle_K = \langle x, T^t y\rangle_H,\ x \in D(T).$$

The definition of adjoint applies just as well when T is replaced by T_0.

We can choose T to be a differential operator in such a way that the resulting space H' is one of the classical Sobolev spaces which is also a Hilbert space. In that case, the restriction T_0 of T can be chosen so that H_0' is a subspace of H' consisting of those members of H' which satisfy zero boundary conditions in some sense (much more variety than this can be accommodated). In the example, T is the derivative operator whose domain consists of the elements of $H^{1,2}([0,1])$. In other cases T might be a gradient operator.

Theorem 5.11. *Suppose $g \in H, w \in H'$, β satisfies (5.16) and*

$$\beta(u) = (1/2)\|u\|_{H'}^2 - \langle g, u\rangle_H,\ u \in H'.$$

Then the element of H' which renders β minimum is the unique solution u to

$$(I + {T_0}^t T)u = g,\ Q_0 u = Q_0 w$$

where Q_0 is as in Theorem 5.10 in its relationship with H', H_0'.

In the example, $(I + {T_0}^t T)$ is the differential operator so that

$$(I + {T_0}^t T)u = u - u''$$

for all u in its domain (without any boundary conditions on its domain - that is it is the maximal operator associated with its expression).

Proof. From Theorem 5.10, the minimum u of β, subject to $Q_0 u = Q_0 w$, may be written

$$u = Q_0 w + M_0 g.$$

It is clear that for u defined in this way $Q_0 u = Q_0 w$, since $R(M_0) \subset R(P_0)$ and $Q_0 = I - P_0$. It remains to show that

$$(I + T_0^t T)u = g.$$

First show that

$$(I + T_0^t T)Q_0 w = 0.$$

To this end, first note that

$$\langle Q_0 w, x\rangle_{H_0'} = 0,\ x \in H_0',$$

since $x = P_0 x, x \in H_0'$. This may be rewritten

$$\langle \left(\begin{smallmatrix} Q_0 w \\ T Q_0 w \end{smallmatrix}\right), \left(\begin{smallmatrix} x \\ T_0 x \end{smallmatrix}\right)\rangle_{H\times K} = 0,\ x \in D(T_0).$$

But this is equivalent to

$$\langle T_0 x, T Q_0 w\rangle_K = \langle x, -Q_0 w\rangle_H,\ x \in D(T_0)$$

and hence

$$T Q_0 w \in D(T_0^t)$$

and

$$T_0^t T Q_0 w = -Q_0 w$$

that is,

$$(I + T_0^t T) Q_0 w = 0.$$

Next show that

$$(I + T_0^t T) M_0 g = g.$$

To do this first note that $M_0 g \in D(T_0)$ since $M_0 g \in H_0'$ and so $T M_0 g = T_0 M_0 g$. Using the definition of M_0,

$$\langle x, g \rangle_H = \langle x, M_0 g \rangle_{H_0'},$$

and so

$$\langle x, g \rangle_H = \langle x, M_0 g \rangle_H + \langle T_0 x, T_0 M_0 g \rangle_K,$$

that is

$$\langle T_0 x, T_0 M_0 g \rangle_K = \langle x, g - M_0 g \rangle_H, \ x \in D(T_0).$$

But this implies that

$$T_0 M_0 g \in D(T_0^t)$$

and

$$T_0^t T_0 M_0 g = g - M_0 g,$$

that is

$$(I + T_0^t T_0) M_0 g = g,$$

and the argument is complete. □

The expression

$$(I + T_0^t T_0) \tag{5.20}$$

is the inverse of M_0 and is called the laplacian associated with the pair (H, H_0'). Similarly the expression

$$(I + T^t T) \tag{5.21}$$

is the laplacian associated with the pair (H, H'). The expression

$$(I + T_0^t T) \tag{5.22}$$

plays the role of maximal operator associated with the triple H, H', H_0'. Theorem 5.11 gives that $R(I + T_0^t T) = H$. One may observe that $N(I + T_0^t T)$ is the orthogonal complement of H_0' in H'.

5.8 Projections for Higher Order Sobolev Spaces

Work of this section is largely taken from [164]. Results in this chapter may be used to specify adjoints related to more general Sobolev spaces $H^{m,2}(\Omega)$ where Ω is an open subset of R^n, $n, m \in Z^+$. For $j = 1, 2, ..., m$ denote by $S(j, n)$ the vector space of all j-linear symmetric functions on R^n. Take $H = L_2(\Omega)$ and

$$K = L_2(\Omega, S(1, n)) \times \cdots \times L_2(\Omega, S(m, n)) \tag{5.23}$$

where $L_2(\Omega, S(j, n))$ denotes the space of square integrable functions from Ω to $S(j, n)$, $j = 1, ..., m$. More precisely, if $e_1, ..., e_n$ denotes any orthonormal basis for R^n and $v \in S(j, n)$, then (see Chapter 22 for more on this topic)

$$\|v\|_{S(j,n)} = (\sum_{p_1=1}^{n} \cdots \sum_{p_j=1}^{n} v(e_{p_1}, ..., v_{p_j})^2)^{1/2}. \tag{5.24}$$

As noted in (Weyl, [226], p 139), [142], this norm is independent of particular choice of orthonormal basis. For $z \in L_2(\Omega, S(j, n))$, define

$$\|z\|_{L_2(\Omega,S(j,n))} = (\int_{\Omega} \|z\|^2_{S(j,n)})^{1/2}. \tag{5.25}$$

Thus the norm on K is the Cartesian product norm on $L_2(\Omega, S(j, n))$, $j = 1, ..., m$. See also [173] in regard to the above construction.

For $u \in C^{(m)}(\Omega)$, denote by Du the m-tuple $(u', u^{(2)}, ..., u^{(m)})$ consisting of the first m Fréchet derivatives of u and take

$$Q = \{(\begin{smallmatrix} u \\ Du \end{smallmatrix}) | u \in C^m(\Omega)\}.$$

From [2], the closure of Q in $H \times K$ is a function W, i.e., no two members of $cl(Q)$ have the same first term. The space $H^{m,2}(\Omega)$ is defined as the set of all first terms of W, with, for $u \in H^{m,2}(\Omega)$,

$$\|u\|_{H^{m,2}}(\Omega) = (\|u\|^2_{L_2(\Omega)} + \|Wu\|^2_K)^{1/2}. \tag{5.26}$$

The orthogonal projection of $H \times K$ onto W will be helpful in later chapters for construction of various Sobolev gradients. Generally, the calculation of such a projection involves the solution of n constant coefficient elliptic equations of order $2m$ on Ω. We will be particularly interested in the numerical solution of such problems.

An alternative to projections for higher order Sobolev spaces comes from Theorem 5.5. This development suggests that, for example, instead of using the transformation M_2 associated with the pair of spaces $L_2(\Omega), H^{2,2}(\Omega)$, one might use M_1^2 where M_1 is the transformation associated with the pair $L_2(\Omega), H^{1,2}(\Omega)$. A numerical use of this is made in Chapter 15 and again in Section 30.8.

Chapter 6
Ordinary Differential Equations and Sobolev Gradients

This chapter shows how a gradient inequality arises for ordinary differential equations. It is indicated how, associated with a nonlinear system, considerations involving the corresponding linearization give a gradient inequality. This gives a clue as to what is taking place in Chapter 9 in which a Nash-Moser type inverse function theorem is given. The essential point of this chapter is revealed by a study of the following simple family of nonlinear ordinary differential equations.

$$u' + q(u) = 0 \text{ on } [0,1],$$

q is a C^2 real function. Corresponding systems could have been treated just as well but the generalization to systems should be clear. Take $H = H^{1,2}([0,1]), K = L_2([0,1])$ and define $F : H \to K$ and $\phi : H \to R$ so that

$$F(u) = u' + q(u),\ u \in H \tag{6.1}$$

and

$$\phi(u) = \frac{1}{2}\|F(u)\|_K^2.$$

Theorem 6.1. *Suppose Q is a bounded subset of H. Then there is $c > 0$ so that*

$$\|(\nabla\phi)(u)\|_H \geq c\|F(u)\|_K,\ u \in Q.$$

Proof. First note that

$$F'(u)h = h' + q'(u)h,\ u, h \in H. \tag{6.2}$$

Then note that if $u, h \in H$,

$$\begin{aligned}\phi'(u)h &= \langle F'(u)h, F(u)\rangle_K \\ &= \langle \begin{pmatrix} h \\ h' \end{pmatrix}, \begin{pmatrix} q'(u)F(u) \\ F(u) \end{pmatrix}\rangle_{K\times K} = \langle h, \pi P\begin{pmatrix} q'(u)F(u) \\ F(u) \end{pmatrix}\rangle_H,\end{aligned}$$

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where $\pi\binom{f}{g} = f,\ f, g \in K$. Thus,

$$\nabla\phi(u) = \pi P \begin{pmatrix} q'(u)F(u) \\ F(u) \end{pmatrix},\ u \in H,$$

where P is the orthogonal projection of $K \times K$ onto

$$\{\begin{pmatrix} u \\ u' \end{pmatrix} : u \in H\},$$

as in Section 5.1.

Now suppose the conclusion to the theorem does not hold. Denote q' by g and denote by $y_1, y_2, ..$ a sequence in Q, so that if $k_n = \frac{F(y_n)}{\|F(y_n)\|}$ and

$$u_n = \pi P\binom{g(y_n)k_n}{k_n},\ n = 1, 2, \ldots,$$

then

$$\lim_{n\to\infty} \|u_n\|_H = 0. \tag{6.3}$$

For each positive integer n, denote by v_n that element of H so that

$$\begin{pmatrix} u_n \\ u_n' \end{pmatrix} + \begin{pmatrix} v_n' \\ v_n \end{pmatrix} = \begin{pmatrix} g(y_n)k_n \\ k_n \end{pmatrix} \tag{6.4}$$

and

$$v_n(0) = 0 = v_n(1). \tag{6.5}$$

Such a decomposition, see Section 5.1, is possible since

$$\{\binom{u}{u'} : u \in H\}^\perp = \{\binom{v'}{v} : v \in H, v(0) = 0 = v(1)\}.$$

Then

$$v_n' = -u_n + g(y_n)k_n \text{ and } k_n = u_n' + v_n$$

so that, with,

$$h_n = -u_n + g(y_n)u_n',\ n = 1, 2, \ldots,$$
$$v_n' = h_n + g(y_n)v_n.$$

It follows that

$$|v_n(t)| \le M_n + c\int_0^t |v_n|,\ n = 1, 2, \ldots,$$

where

$$M_n = \sup_{t\in[0,1]} \int_0^t |h_n| \text{ and } c \ge |g(y_n)|,\ n = 1, 2, \ldots,$$

By Gronwall's inequality,

$$|v_n(t)| \le M_n \exp(ct),\ t \in [0,1],\ n = 1, 2, \ldots,$$

so that

$$\lim_{n\to\infty} \|v_n\|_{sup} = 0.$$

This gives a contradiction since

$$1 = \|k_n\|_K = \|u_n' + v_n\|_K \le \|u_n'\|_K + \|v_n\|_K \to 0 \text{ as } n \to \infty,$$

and thus the theorem is established. □

Note that the existence of a gradient inequality does not by itself imply convergence of continuous steepest descent to a solution. Indeed, such a general conclusion is not possible since (6.1) may well not have a solution on all of $[0,1]$. The existence of a gradient inequality on bounded sets can be used in conjunction with results in Chapter 4 in exploring possibilities for (6.1).

As mentioned, this theorem generalizes immediately to systems of ordinary differential equations in a finite dimensional space. More intriguingly, it seems likely to this writer that there are substantial generalizations to the above to systems of partial differential equations.

Chapter 7
Convexity and Gradient Inequalities

It has long been recognized that convexity of ϕ, from a Hilbert space H to R, is an important consideration in the study of steepest descent. Convexity of a function ϕ in the neighborhood of a zero of ϕ is indicative of convergence of continuous steepest descent if the start of the descent is close enough to that zero. For the next theorem take ϕ to be, at each point of H, convex in the gradient direction at that point. More specifically there is:

Theorem 7.1. *Suppose ϕ is a nonnegative $C^{(2)}$ function on H for which there is $\epsilon > 0$ such that*

$$\phi''(x)((\nabla\phi)(x), (\nabla\phi)(x)) \geq \epsilon\|(\nabla\phi)(x)\|_H^2,\ x \in H. \tag{7.1}$$

Suppose also that $x \in H$, $(\nabla\phi)(x) \neq 0$ and (4.2) holds. Then

$$u = \lim_{t\to\infty} z(t) \text{ exists and } (\nabla\phi)(u) = 0.$$

Proof. Define $g = \phi(z)$ where for $x \in H$, z satisfies (4.2). Note that $g' = \phi'(z)z' = -\|(\nabla\phi)(z)\|_H^2$ and

$$g'' = 2\langle(\nabla\phi)'(z)z', z'\rangle_H.$$

Note also that if each of $h, k, y \in H$ then

$$\phi''(y)(h, k) = \langle(\nabla\phi)'(y)h, k\rangle_H.$$

Using (7.1),

$$g''(t) = 2\langle(\nabla\phi)'(z(t))z'(t), z'(t)\rangle_H \geq 2\epsilon\|z'(t)\|_H^2 = -2\epsilon g'(t),\ t \geq 0.$$

and so

$$\frac{-g''(t)}{g'(t)} \geq 2\epsilon,\ t \geq 0$$

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Hence

$$-\ln \frac{-g'(t)}{-g'(0)} \geq 2\epsilon t,\ t \geq 0.$$

and consequently,

$$0 \leq -g'(t) \leq -g'(0)\exp(-2\epsilon t), t \geq 0 \tag{7.2}$$

and

$$\lim_{t\to\infty} g'(t) = 0.$$

From (7.2) it follows that if $0 \leq a < b$, then

$$g(a) - g(b) \leq (-g'(0))(\exp(-2\epsilon a) - \exp(-2\epsilon b))/(2\epsilon).$$

But

$$g'(t) = -\|z'(t)\|_H^2, t \geq 0,$$

and so

$$-\int_a^b g' = \int_a^b \|z'\|_H^2, 0 < a < b.$$

Therefore

$$g(a) - g(b) = \int_a^b \|z'\|_H^2 \text{ and hence}$$

$$\int_a^b \|z'\|_H^2 \leq (-g'(0))(\exp(-2\epsilon a) - \exp(-2\epsilon b))/(2\epsilon).$$

Therefore,

$$-g'(0)\exp(-2\epsilon a)/(2\epsilon) \geq \int_a^{a+1} \|z'\|_H^2 \geq (\int_a^{a+1} \|z'\|_H)^2.$$

Hence, $\int_0^\infty \|z'\|_H$ exists and consequently

$$u = \lim_{t\to\infty} z(t)$$

exists. Since $\lim_{t\to\infty} g'(t) = 0$ and $-\|(\nabla\phi)(z(t))\|_H^2 = g'(t)$, it follows that

$$(\nabla\phi)(u) = \lim_{t\to\infty} (\nabla\phi)(z(t)) = 0.$$

□

The above is close to arguments found in [208]. An alternate argument is in [196, 200]. In these two references, the convexity condition (7.1) is shown to imply a gradient inequality and hence one has convergence for continuous steepest descent in the presence of convexity. Even without differentiability assumptions on ϕ, a subgradient of ϕ may be defined. This subgradient becomes a monotone operator. The theory of one parameter semigroups of nonlinear contraction mappings on Hilbert space then applies. The interested reader might see [25] for such developments. It is emphasized that for many problems of interest in the present context, ϕ is not convex. The preceding theorem is included mainly for comparison.

Note, however, the following connection between convexity conditions and gradient inequalities. The following was essential pointed out by J.P. Holmes in a private communication.

Theorem 7.2. *Suppose F is a $C^{(2)}$ function from H to K, $u \in H$, $F(u) = 0$ and $s, d > 0$ so that*

$$\|F'(x)^*F(x)\|_H \geq d\|F(x)\|_K, \ \textit{if } \|x-u\|_H \leq s.$$

Then there exist $r, \epsilon > 0$ so that

$$\phi''(x)((\nabla\phi)(x),(\nabla\phi)(x)) \geq \epsilon\|(\nabla\phi)(x)\|_H^2 \ \textit{if } \|x-u\|_H < r.$$

Lemma 7.3. *Suppose that $T \in L(H,K)$, $y \in K$, $y \neq 0$, $d > 0$ and $\|T^*y\|_H \geq d\|y\|_K$. Then*

$$\|TT^*y\|_K \geq (d^2/|T^*|)\|T^*y\|_H.$$

Proof. (Lemma 7.3) First note that

$$\begin{aligned}\|TT^*y\|_K &= \sup_{\|k\|_K=1} \langle TT^*y, k\rangle_K \\ &\geq \langle TT^*y, \frac{1}{\|y\|_K}y\rangle_K \\ &= \frac{\|T^*y\|_H^2}{\|y\|_K} \geq d^2\|y\|_K.\end{aligned}$$

Hence

$$\frac{\|TT^*y\|_K}{\|T^*y\|_H} = \frac{\|TT^*y\|_K}{\|y\|_K}\frac{\|y\|_K}{\|T^*y\|_H} \geq \frac{d^2}{|T^*|}$$

since

$$\frac{\|T^*y\|_H}{\|y\|_K} \leq |T^*|.$$

□

Proof. (Of Theorem 7.2) Note that if $x, h \in H$ then

$$\phi''(x)(h,h) = \|F'(x)h\|_K^2 + \langle F''(x)(h,h), F(x)\rangle_K.$$

Choose $r_1, M_1, M_2 > 0$ so that if $\|x-u\|_H \le r_1$, then

$$|F'(x)| \le M_1 \text{ and } |F''(x)| \le M_2.$$

Pick $r > 0$ so that $r \le \min(s, r_1)$ and

$$\|F(x)\|_K \le \alpha \equiv \frac{d^2}{2M_1M_2} \text{ if } \|x-u\|_H \le r.$$

Then using the lemma and taking x, h so that

$$\|x-u\|_H \le r \text{ and } \quad h = (\nabla\phi)(x),$$

$$\|F'(x)^*h\|_K \ge \frac{d^2}{M_1}\|(\nabla\phi)(x)\|_H$$

and

$$|\langle F''(x)(h,h), F(x)\rangle_K| \le M_2\alpha\|(\nabla\phi)(x)\|_H^2.$$

Hence

$$\phi''(x)(h,h) \ge (\frac{d^2}{M_1} - M_2\alpha)\|(\nabla\phi)(x)\|_H^2 = \epsilon\|(\nabla\phi)(x)\|_H^2,$$

where

$$\epsilon \equiv \frac{d^2}{M_1} - M_2\alpha = \frac{d^2}{2M_1} > 0.$$

□

Another result for which existence of an ω-limit point implies convergence is the following. The chapter on convexity in [59] influenced the formulation of this result.

Theorem 7.4. *Under the hypothesis of Theorem 4.1, suppose that $x \in H$ and z satisfies (4.2). Suppose also that u is an ω-limit point of z at which ϕ is locally convex. Then*

$$u = \lim_{n\to\infty} z(t) \text{ exists}$$

and $(\nabla\phi)(u) = 0$.

Proof. Suppose that $\{t_i\}_{i=1}^\infty$ is an increasing unbounded sequence of positive numbers so that

$$u = \lim_{i\to\infty} z(t_i) \tag{7.3}$$

but that it is not true that

$$u = \lim_{t\to\infty} z(t). \tag{7.4}$$

Then z is not constant and it must be that $\phi(z)$ is decreasing. Define α so that

$$\alpha(t) = \frac{\|z(t) - u\|_H^2}{2},\ t \geq 0.$$

Note that

$$\begin{aligned}\alpha'(t) &= \langle z'(t), z(t) - u\rangle_H = -\langle (\nabla\phi)(z(t)), z(t) - u\rangle_H \\ &= \langle (\nabla\phi)(z(t)), u - z(t)\rangle_H,\ t \geq 0.\end{aligned}$$

If for some $t_0 \geq 0, \alpha'(t) \leq 0$ for all $t \geq t_0$, then (7.4) would follow in light of (7.3). So suppose that for each $t_0 \geq 0$ there is $t > t_0$ so that $\alpha'(t) > 0$. For each positive integer n, denote by s_n the least number so that $s_n \geq t_n$ and so that if $\epsilon > 0$ there is $t \in [s_n, s_n + \epsilon]$ such that $\alpha'(t) > 0$. Note that

$$\phi(z(s_n)) \leq \phi(z(t_n)),\ n = 1, 2, \ldots .$$

Denote by $\{q_n\}_{n=1}^\infty$ a sequence so that $q_n > s_n, \alpha'(q_n) > 0$ and

$$\|z(s_n) - z(q_n)\| < \frac{1}{n},\ n = 1, 2, \ldots$$

and note that $\lim_{n\to\infty} z(q_n) = u$ since

$$\|z(s_n) - u\|_H \leq \|z(t_n) - u\|_H,\ \|z(s_n) - z(q_n)\|_H < \frac{1}{n},\ n = 1, 2, \ldots$$

and $\lim_{n\to\infty} z(t_n) = u$.

Now if n is a positive integer,

$$0 < \alpha'(q_n) = \langle (\nabla\phi)(z(q_n)), u - z(q_n)\rangle_H = \phi'(z(q_n))(u - z(q_n))$$

and so there is $p_n \in [z(q_n), u]$ so that $\phi(p_n) > \phi(z(q_n))$. But $\phi(z(q_n)) > \phi(u)$ since $\phi(z)$ is decreasing and (7.3) holds. Thus $\phi(z(q_n)) < \phi(p_n) > \phi(u)$. Since p_n is between $z(q_n)$ and u, it follows that ϕ is not convex in the ball with center u and radius $\|z(q_n) - u\|_H$. But $\lim_{n\to\infty} \|z(q_n) - u\|_H = 0$ so ϕ is not locally convex at u, a contradiction. Thus the assumption that (7.4) does not hold is false and so (7.4) holds. Since

$$\int_0^\infty \|(\nabla\phi)(z)\|^2 < \infty,$$

it follows that $(\nabla\phi)(u) = 0$. □

Chapter 8
Boundary and Supplementary Conditions

8.1 Introduction

Many systems of differential equations may be placed in one of the following settings: For a C^1 function $\phi : H \to R$ find $u \in H$ so that either

$$\nabla\phi(u) = 0 \tag{8.1}$$

or

$$\phi(u) = 0. \tag{8.2}$$

Under some set of additional restrictions on a solution u to (8.1) or (8.2), there may be a unique solution which satisfies these conditions. How might one specify such conditions? There is, of course, a vast literature which gives definitive answers to various cases (ordinary differential equations, elliptic, hyperbolic, parabolic partial differential equations for instance) but in any substantial generality, this question is certainly one of the most difficult ones in mathematics. It is so difficult that the problem doesn't even have a name.

For many systems of ordinary differential equations, specifying initial conditions at some point specifies a unique solution. For partial differential equations on a region Ω in some Euclidean space, conditions for a unique solution are commonly given on at least part of the boundary of Ω. However even in some linear problems (for example, the Tricomi equation in Chapter 15) conditions for a unique solution seem not to be known.

This question will arise a number of times in this book. Chapters 14, 15,16,17,19,20 and in particular in the survey Chapter 30 where there are examples dealing with the hyperbolic Monge-Amper equation, Ginzburg-Landau equation without a penalty term and others.. In this last instance, a solution is a function u from the computational region $\Omega \subset R^3$ into R^3. A supplementary condition there is that $\|u(x)\| = 1,\ x \in \Omega$, certainly far removed from a 'boundary condition'. The present chapter is an introduction to a point of view on the subject of supplementary conditions for partial differential equations. We prefer the term 'supplementary conditions'

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to 'boundary conditions' since there are many ways to impose conditions on a function other than conditions on a boundary.

Suppose each of H, S is a Hilbert space and $\phi : H \to R$, $B : H \to S$ each a C^1 function. Consider the problem of finding $u \in H$ so that

$$(\nabla\phi)(u) = 0 \text{ and } B(u) = 0. \tag{8.3}$$

Think of the second equation as specifying a supplementary condition on u and the first equation as specifying an equation to be solved. In many cases of interest, $(\nabla\phi)(u) = 0$ implies $\phi(u) = 0$, in particular in the presence of a gradient inequality for ϕ.

For an example, define

$$\phi(u) = \frac{1}{2}\int_0^1 (u' - u)^2, \; u \in H^{1,2}([0,1])) \tag{8.4}$$

and take

$$B(u) = u(0) - 1, \; u \in H^{1,2}([0,1])). \tag{8.5}$$

For this choice of ϕ and B, the problem (8.1) becomes that of finding $u \in H^{1,2}([0,1])$ so that

$$u' - u = 0, \; u(0) = 1. \tag{8.6}$$

Note that here $S = R$,

A gradient is sought that takes both ϕ and B into account. Specifically seek $\nabla_B\phi$ so that if $x \in H$ and

$$z(0) = x, \; z'(t) = -(\nabla_B\phi)(z(t)), \; t \geq 0, \tag{8.7}$$

then

$$B(z(t)) = B(x), \; t \geq 0. \tag{8.8}$$

Hence B provides an invariant for solutions z to (8.7), and also that

$$u = \lim_{t\to\infty} z(t)$$

exists and

$$(\nabla\phi)(u) = 0.$$

In particular, if $x \in H$, $B(x) = 0$ and (8.8) holds, then $B(u) = 0$, that is, u satisfies the required supplementary condition if $u = \lim_{t\to\infty} z(t)$.

Sections to follow in this chapter develop a gradient which can be used to solve (8.3). The present chapter might be read in connection with the discussion of supplementary conditions for general Lax-Milgram systems in Section 5.6.

8.2 Orthogonal Projection onto a Null Space

Lemma 8.1. *Suppose that each of H, V is a Hilbert space and $Q \in L(H, V)$. Suppose also that $(QQ^*)^{-1}$ exists and belongs to $L(V, H)$. Then the orthogonal projection J of V onto $N(Q)$ is given by*

$$J = I - Q^*(QQ^*)^{-1}Q.$$

Proof. Note that $Q^*(QQ^*)^{-1}Q$

- is idempotent,
- is symmetric,
- has range a subset of $R(Q^*)$,
- is fixed on $R(Q^*)$.

These four properties imply that $Q^*(QQ^*)^{-1}Q$ is the orthogonal projection onto $R(Q^*)$. Thus J is its complementary projection, i.e., the orthogonal projection onto

$$N(Q) = R(Q^*)^{\perp}.$$

□

In intended applications, $Q = B'(u)$ where B, u are as in (8.3). What is the form of Q^* in such cases? The start of an answer is follows.

8.3 Projected Sobolev Gradients, Linear Case

We return to the general setting of (8.3) but first deal with the case of B linear. Suppose that each of H and S is a Hilbert space and $B \in L(H, S)$. Denote $N(B)$ by H_0. Suppose further that $\phi : H \to R$ is a C^1 function. Pick $w \in H$. Define $\alpha : H_0 \to R$ by

$$\alpha(x) = \phi(w + x),\ x \in H_0. \tag{8.9}$$

The Sobolev gradient $\nabla\alpha$ of α is the function on H_0 such that

$$\alpha'(x)h = \langle h, (\nabla\alpha)(x)\rangle_{H_0},\ x, h \in H_0.$$

Now $\nabla\alpha$ is calculated in terms of ϕ. So,

$$\alpha'(x)h = \phi'(w + x)h = \langle h, (\nabla\phi)(w + x)\rangle_H,\ x, h \in H_0. \tag{8.10}$$

Denote by P_B the orthogonal projection onto $N(B)$. Then from (8.10), since $P_B h = h,\ h \in N(B)$,

$$\alpha'(x)h = \langle P_B h, (\nabla\phi)(w + x)\rangle_H = \langle h, P_B(\nabla\phi)(w + x))\rangle_{H_0},\ x, h \in H_0.$$

Hence

$$(\nabla\alpha)(x) = P_B(\nabla\phi)(w+x),\ x \in H_0. \tag{8.11}$$

Here is some explanation to go with steps above: The gradient $\nabla\phi$ doesn't have range, necessarily, in H_0 and so it can't give a representation of α'. This is a standard feature of optimization theory: we have turned a constrained problem into an unconstrained one. Note, however, that α depends on a choice of w in (8.9). For the gradient $\nabla\alpha$, results of Chapter 4 that are set in an abstract Hilbert space are available.

8.4 Projected Gradients, Nonlinear Case

For B nonlinear and C^1, a construction of a Sobolev gradient for (8.3) follows a similar pattern as in the case B is linear. The main difference is that in the nonlinear case P_B is a function so that for $x \in H$, $P_B(x)$ is the orthogonal projection of H onto $N(B'(x))$. Accordingly, define

$$(\nabla_B\phi)(x) = P_B(x)(\nabla\phi)(x)),\ x \in H$$

where $\nabla\phi$ is the Sobolev gradient of ϕ taken without regard to B. Assuming that P_B is C^1, $x \in H$ and

$$z(0) = x,\ z'(t) = -(\nabla_B\phi)(z(t)),\ t \geq 0. \tag{8.12}$$

Then,

$$(B(z))'(t) = B'(z(t))(\nabla_B\phi)(z(t)) = B'(z(t))P_B(z(t))(\nabla\phi)(z(t)) = 0,\ t \geq 0$$

and so if $u = \lim_{t\to\infty} z(t)$, then $B(u) = B(x)$ and hence $B(u) = 0$ granted that $B(x) = 0$ for steepest descent starting at x.

8.5 Explicit Form for a Projected Gradient

Take $H = H^{1,2}([0,1]),\ v \in R$ and $K = L_2([0,1])$. Define ϕ and B so that

$$\phi(y) = \frac{1}{2}\int_0^1 (y' - y)^2,\ B(y) = y(0) - 1,\ y \in H. \tag{8.13}$$

Then if $y \in H$ is a solution to

$$\phi(y) = 0,\ B(y) = 0,$$

it also satisfies (8.6).

An expression for a Sobolev gradient for this problem will be found and will be called

$$\nabla_Q \phi,$$

with Q denoting the common value of the range of B'.

Note that

$$Qf = f(0),\ f \in H.$$

Again, C and S are defined by

$$C(t) = \cosh(t),\ S(t) = \sinh(t),\ j(t) = t,\ t \in R.$$

Theorem 8.2. *With ϕ and B defined in (8.13),*

$$((\nabla_Q \phi)(y))(t) = y(t) - [y(1)S(t) + y(0)C(1-t)]/C(1),\ t \in [0,1].$$

There are several steps to prove this theorem. The first one calculates $\nabla\phi$.

Lemma 8.3. *If $y \in H$, then*

$$((\nabla\phi)(y))(t) = y(t) - [y(1)C(t) - y(0)C(1-t)]/S(1),\ t \in [0,1]. \tag{8.14}$$

Proof. Note that

$$\phi'(y)h = \int_0^1 (h'-h)(y'-y), = \langle \binom{h}{h'}, \binom{y-y'}{y'-y} \rangle = \langle \binom{h}{h'}, P\binom{y-y'}{y'-y} \rangle,\ h, y \in H,$$

where P is the orthogonal projection defined in (5.8). Since $P\binom{y}{y'} = \binom{y}{y'}$,

$$(\nabla\phi)(y) = y - u$$

where $\binom{u}{u'} = P\binom{y'}{y}$.

Using (5.3),

$$\begin{aligned} u(t) &= (C(1-t)\int_0^t (Cy' + Sy) + C(t)\int_t^1 (C(1-j)y' - S(1-j)y))/S(1) \\ &= (C(1-t)(C(t)y(t) - C(0)y(0))) \\ &\quad + C(t)(C(0)y(1) - C(1-t)y(t)))/S(1) \\ &= (C(t)y(1) - C(1-t)y(0))/S(1),\ t \in [0,1], \end{aligned}$$

since $(Cy)' = Cy' + Sy$ and $(C(1-j)y)' = C(1-j)y' - S(1-j)y$. This gives Lemma 8.3. □

Recall now that

$$(\nabla_Q \phi)(y) = P_Q(y)(\nabla \phi)(y),\ y \in H.$$

Next we seek an explicit expression for $P_Q(y)h$ where $h, y \in H$. One can arrive at this result using considerations following (8.21), but here we have chosen to so by a direct calculation:

Denote $N(Q)$ by H_0, a subspace of H which has the same norm as H:

$$H_0 = \{f \in H : f(0) = 0\}.$$

The next lemma gives us an expression for Q^*.

Lemma 8.4. *Suppose $Qh = h(0)$, $h \in H$. Then*

$$(Q^* w)(t) = wC(1-t)/S(1),\ t \in [0,1],\ w \in R. \tag{8.15}$$

Proof. Suppose $w \in R$. Then there is a unique $f \in H$ so that

$$h(0)w = \langle Qh, w\rangle_R = \langle h, f\rangle_H,\ h \in H.$$

To determine this element f, note that if $f \in C^2([0,1])$, then

$$\langle h, f\rangle_H = \int_0^1 (hf + h'f') = \int_0^1 h(f - f'') + h(1)f'(1) - h(0)f'(0)$$

and so if

$$wh(0) = \langle h, f\rangle_H,\ h \in H,$$

it must be that

$$f - f'' = 0, f'(1) = 0 \text{ and } f'(0) = -w. \tag{8.16}$$

It is an exercise in ordinary differential equations to find f satisfying (8.16). Such an f is given by (8.15). □

Lemma 8.5. *Let J be the orthogonal projection of H onto $N(Q)$. Then*

$$(Jh)(t) = h(t) - h(0)C(1-t)/C(1),\ h \in H_0, t \in [0,1].$$

Proof. Use Lemma 8.3 to calculate $Q^*(QQ^*)^{-1}Q$: If $w \in R$,

$$QQ^* w = (Q^* w)(0) = wC(1)/S(1)$$

and so

$$(QQ^*)^{-1} w = wS(1)/C(1).$$

Hence if $h \in H$,

$$
\begin{aligned}
(Q^*(QQ^*)^{-1}Qh)(t) &= ((QQ^*)^{-1}Q^*Qh)(t) \\
&= h(0)(S(1)/C(1))(C(1-t)/S(1)) \\
&= h(0)C(1-t)/C(1),\ t \in [0,1].
\end{aligned}
$$

The conclusion follows immediately. □

Proof. (Of Theorem 8.2). Note that $P_Q(y) = J$ for any $y \in H$. A direct calculation using Lemmas 8.3 and 8.4 yields

$$
\begin{aligned}
((\nabla Q\phi)(y))(t) &= (J((\nabla\phi)(y)))(t) \\
&= y(t) - [y(1)S(t) + y(0)C(1-t)]/C(1),\ t \in [0,1].
\end{aligned}
$$

□

A reader may verify that if $(\nabla_Q\phi)(y) = 0$, then

$$y(t) = y(0)\exp(t),\ t \in [0,1],$$

so that an iteration that preserves $y(0)$ and yields a zero of $\nabla_Q\phi$ has converged to the expected solution. Next are two iteration methods with this gradient, one continuous and one discrete, for which one can observe that this happens. In Chapter 10 there is a somewhat different way to arrive at $\nabla_Q\phi$.

8.6 Continuous *vs* Discrete Steepest Descent

For the simple problem in the previous section, one can carry out explicitly both continuous and discrete steepest descent for simple cases. Similar exercises can be done with $\nabla_Q\phi$ replaced by $\nabla\phi$, the Sobolev gradient taken without regard to boundary conditions.

For the vast majority of problems, iterations are a matter of a computer code, but a reader may find it interesting to carry out some steps by hand for this simple example.

Exercise 8.6. Using results of Chapter 3, solve

$$z(0) = v \in R,\ z'(t) = -(\nabla_Q\phi)(z(t),\ t \geq 0.$$

Show that $u = \lim_{t\to\infty} z(t)$ exists, $u(0) = v$, and $u' - u = 0$.

Exercise 8.7. Use $\nabla_Q\phi$ in discrete steepest descent. Pick $v \in R$, choose $f_0 \in H$ such that $f_0(0) = v$ and $\{f_m\}_{m=1}^{\infty}$ so that

$$f_{m+1} = f_m - \delta_m(\nabla_Q \phi),\ m = 0, 1, \ldots,$$

where δ_m is chosen as the number δ so that

$$\frac{1}{2}\|f_m - \delta(\nabla_Q \phi)(f_m)\|_H^2$$

is minimum (this is a simple quadratic equation to solve for δ).

Then observe that $\{f_m\}_{m=1}^{\infty}$ converges to $u \in H$ such that $u(0) = v$ and $u' - u = 0$.

Theorems in the second part of Chapter 4 all have appropriate generalizations in which $\nabla_Q \phi$ replaces $\nabla \phi$. More on numerical solutions appear in later chapters.

8.7 A Finite Dimensional Example for Adjoints

This section gives a preview for Chapter 10 where numerical calculations using Sobolev gradients are discussed more fully.

For a positive integer $n > 2$ take H_n to be the finite dimensional Hilbert space whose points are those of R^{n+1} but, for $y = (y_0, y_1, \ldots, y_n)$,

$$\|y\|_{H_n}^2 = \sum_{k=0}^{n} y_k^2 + \sum_{k=1}^{n} (\frac{1}{\delta}(y_k - y_{k-1}))^2, \tag{8.17}$$

making H_n a finite dimensional version of the Sobolev space $H^{1,2}([0, 1])$, where $\delta = \frac{1}{n}$, the mesh size of the partition

$$(\frac{0}{n}, \frac{1}{n}, \ldots, \frac{n}{n})$$

of $[0, 1]$. Of course this norm is equivalent to the Euclidean norm, but as seen in Chapter 2, norm choice can make a great difference in calculations.

Define $D : H_n \to R^{2n+1}$ by

$$Dy = (y, \frac{1}{\delta}((y_1 - y_0), \ldots, (y_n - y_{n-1}))), y \in H_0. \tag{8.18}$$

Thus for $y \in H_n$,

$$\|y\|_{H_n}^2 = \|Dy\|_{R^{2n+1}}^2.$$

Pick k in $\{0, 1, \ldots, n\}$. Take $B_k : H_n \to R$ so that

$$B_k y = y_k,\ y \in H_n.$$

Then $B_k^* : R \to H_n$. The following gives an expression for B_k^*:

Lemma 8.8. *$B_k^* x = (D^t D)^{-1} x e_k = x(D^t D)^{-1} e_k$ where e_k is the $k-th$ standard basis vector in R^{n+1}, $k = 0, 1, \ldots, n$.*

Proof. If $x \in R$ then

$$xy(k) = \langle x, B_k y\rangle_R = \langle y, xe_k\rangle_{R^{n+1}} = \langle y, D^t D(D^t D)^{-1} xe_k\rangle_{R^{n+1}}$$
$$= \langle Dy, D(D^t D)^{-1} xe_k\rangle_{R^{2n+1}} = \langle y, (D^t D)^{-1} xe_k\rangle_{R^n},\ y \in H_n,$$

and so the conclusion follows. □

The transformation $(D^t D)^{-1}$ is an example of a transformation M arising from Theorem 5.4. To see this, replace H in Theorem 5.4 by R^{n+1}, with the standard norm, and H' in Theorem 5.4 by the space H_n of Lemma 8.5.

A MatLab code gives $(D^t D)^{-1} e_k$ for $n = 100$ with $k = 33$ in Figure 8.1 and $k = 50$ in Figure 8.2. These are close approximations to two cross-sections of a relevant two dimensional Green's function, as follows. Consider $H = L_2([0,1]), H' = H^{1,2}([0,1])$ and suppose $g \in H'$, $f \in H$. Then

$$\langle g, f\rangle_H = \langle \begin{pmatrix} g \\ g' \end{pmatrix}, \begin{pmatrix} f \\ 0 \end{pmatrix}\rangle_{H^2} = \langle \begin{pmatrix} g \\ g' \end{pmatrix}, P\begin{pmatrix} f \\ 0 \end{pmatrix}\rangle_{H^2} = \langle g, \pi P\begin{pmatrix} f \\ 0 \end{pmatrix}\rangle_{H^2}$$

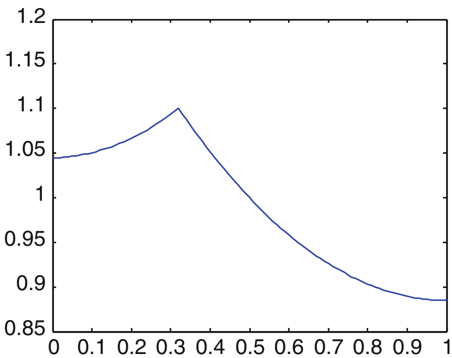

Fig. 8.1 n=100, k=33

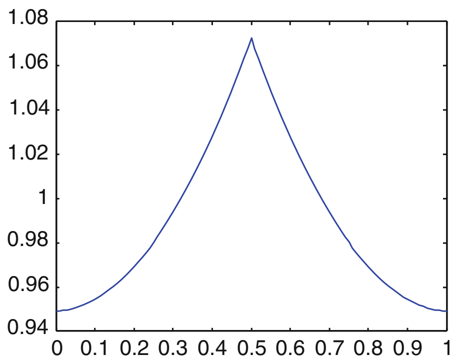

Fig. 8.2 n=100, k=50

where P is the orthogonal projection of H^2 onto

$$\{\begin{pmatrix} h \\ h' \end{pmatrix} : h \in H'\} \tag{8.19}$$

and $\pi\binom{r}{s} = r,\ r, s \in H$. (see (5.3)).

In the development up to Theorem 5.4, there is uniquely $M : H \to H'$ so that

$$\langle g, f\rangle_H = \langle g, Mf\rangle_{H'},\ f \in H, g \in H'. \tag{8.20}$$

Putting (8.19) and (8.20) together,

$$Mf = \pi P\begin{pmatrix} f \\ 0 \end{pmatrix},\ f \in H.$$

Thus from (5.3) one has that if $K : [0,1] \times [0,1] \to R$ is given by

$$K(t,s) = \begin{cases} C(1-t)C(s)/S(1) & \text{if } 0 \le t \le s \\ C(t)C(1-s)/S(1) & \text{if } s < t \le 1. \end{cases}$$

$(C = \cosh, S = \sinh)$ then

$$(Mf)(t) = \int_0^1 K(t,\cdot)f,\ t \in [0,1]. \tag{8.21}$$

The transformation $(D^tD)^{-1}$ above is a finite dimensional transformation which approximates the embedding operator M.

Plots of $K(.33,\cdot)$ and $K(.5,\cdot)$ match well Figures 8.1 and 8.2 respectively, as they should. To see why, for some $k \in 0, 1, \ldots, n$, pick a sequence of nonnegative continuous functions $\{f_m\}_{m=1}^{\infty}$ on $[0,1]$ so that

- The length of the support of f_m converges to zero as $m \to \infty$.
- The support of f_m contains k/n.
- $\int_0^1 f_m = 1,\ m = 1, 2, \ldots$.

Then

$$\lim_{m\to\infty} (Mf_m)(t) = K(t, k/n).$$

where M is from (8.21). I suppose I might have said, 'let f in (8.21) be the Dirac Delta function centered at k/n'. This is an indication that (8.21) is a limiting case, as $m \to \infty$, of a sequence of problems as in the first part of this section.

Having B_k for some $k \in 0, 1, \ldots, n$, it is an exercise to derive an expression for $J = I - B_k^*(B^kB_k^*)^{-1}B_k$ and thus project H_n onto $N(B_k)$.

Two other examples follow. In each there is a supplementary condition function $B : H_n \to S$ for some vector space S. The key to finding the orthogonal projection of onto $N(B)$ is, as above, the calculation of $B^* : S \to H_n$.

For the first example, choose $S = R$, n an even positive integer and $B : H_n \to R$ given by

$$B(y) = y(0) + y(n/2) + y(n),\ y = (y_0, y_1, \ldots, y_n) \in H_n.$$

To calculate $B^* : R \to H_n$, observe that if $x \in R$ and $y = y_0, y_1, \ldots, y_n \in H_n$. then $B^*x = g \in H_n$ so that

$$\begin{aligned}\langle By, x\rangle_R &= x(y_0 + y_{n/2} + y_n) = \langle y, g\rangle_{H_n}\\ &= \langle Dy, Dg\rangle = \langle y, D^t Dg\rangle_{R^{n+1}}.\end{aligned}$$

Hence it must be that

$$\hat{x} = D^t Dg \tag{8.22}$$

where

$$\hat{x} = (x, 0, \ldots, 0, x, 0, \ldots, 0, x),$$

in which $'x'$ appears in the above in positions $0, n/2, n$. Then g is obtained from (8.22) by solving that linear system.

For another example, take $B : H_n \to R^3$ given by

$$B(y) = (y(0), y(n/2), y(n)),\ y = (y_0, y_1, \ldots, y_n) \in H_n.$$

In this case, for $(r, s, t) \in R^3$, to find

$$B^* \begin{pmatrix} r \\ s \\ t \end{pmatrix},$$

solve the linear system

$$\hat{z} = D^t Dg$$

for g where $\hat{z}$ is the member of R^3 with r, s, t respectively in positions $0, n/2, n$ and zeros elsewhere. See [229] and references contained therein for a perspective on Green's functions and ordinary differential equations.

8.8 Approximation of Projected Gradients

We now turn now to another matter concerning supplementary conditions. This development is given in a finite dimensional setting even though one surely exists also in function spaces. Results will be illustrated here in one dimension (see [147] for some higher dimensional results). It will be shown how to weight finite dimensional versions of Sobolev spaces so that gradients that respect supplementary conditions are approximated, as weights approach infinity, by gradients taken with respect to a succession of weighted spaces. An application of this idea is in Chapter 15, which deals with the Tricomi equation. This writer's use of such a succession of weighted spaces started in the 1970s. This predates the use of projections P_Q as in previous sections of this chapter.

A general question: For a given function ϕ on a Sobolev space, how might the Sobolev gradient of ϕ change if the Sobolev metric is perturbed. In place of an attempt at a general discussion of this issue, a discussion is focused on the simplest case, a one-dimensional setting in which just one point has a weight.

Denote by n a positive integer greater than two. Denote $\frac{1}{n}$ by γ_n, by λ a positive number not less than one and by H_λ the vector space whose points are those of R^{n+1} but for $x = (x_0, x_1, \ldots, x_n) \in R^{n+1}$,

$$\|x\|_\lambda^2 = \lambda x_0^2 + [\sum_{i=1}^{n} (\frac{x_i - x_{i-1}}{\gamma_n})^2 + x_i^2].$$

The inner product associated with this norm is denoted by

$$\langle \cdot, \cdot \rangle_\lambda$$

The space H_1 is just a finite dimensional version of $H^{1,2}([0,1])$. The pair (R^{n+1}, H_λ) is an example of a pair of Hilbert spaces dealt with by Theorem 5.4. Denote by M_λ the transformation so that if $x, y \in R^{n+1}$, then

$$\langle x, y \rangle_{R^{n+1}} = \langle x, M_\lambda y \rangle_\lambda. \tag{8.23}$$

Denote by P the orthogonal projection of R^{n+1} so that if $x = (x_0, x_1, \ldots, x_n) \in R^{n+1}$, then

$$Px = (0, x_1, \ldots, x_n).$$

Note that if $x, y \in R^{2n+1}$ then

$$\langle x, y \rangle_\lambda = \lambda x_0 y_0 + \sum_{k=1}^{n} (x_k y_k + \frac{x_k - x_{k-1}}{\gamma_n} \frac{y_k - y_{k-1}}{\gamma_n}). \tag{8.24}$$

Suppose that $\phi : R^{n+1} \to R$ is a C^1 function and $\lambda \geq 1$. Denote by $\nabla_\lambda \phi$ the function on R^{n+1} so that, with $(\nabla \phi)(u)$ denoting the ordinary gradient of ϕ at u,

$$\begin{aligned} \phi'(u)h &= \langle h, (\nabla \phi)(u) \rangle_{R^{n+1}} \\ &= \langle h, (\nabla_\lambda \phi(u)) \rangle_\lambda, \ h \in R^{n+1}. \end{aligned}$$

Fix $u \in R^{n+1}$. From (8.24), with $g = (g_0, g_1, \ldots, g_n) = (\nabla_\lambda \phi)(u)$,

$$\begin{aligned}\phi'(u)h &= (\lambda - 1)x_0 g_0 + \langle h, D^t D g\rangle_{R^{n+1}} \\ &= \langle((\lambda-1)P + I)h, D^t D g\rangle_{R^{n+1}} \\ &= \langle h, ((\lambda-1)P + I)D^t D g\rangle_{R^{n+1}},\ h \in R^{n+1}.\end{aligned}$$

Thus,

$$(\nabla_\lambda \phi)(u) = ((\lambda-1)P + I)D^t D)^{-1}(\nabla\phi)(u)). \tag{8.25}$$

The indicated inverse in (8.25) exists since $D^t D \geq I$ is symmetric, and the projection P is nonnegative and symmetric. Using (8.23),

$$(\nabla_\lambda \phi)(u) = M_\lambda(\nabla\phi)(u),\ u \in R^{n+1}.$$

Now determine limiting properties of M_λ as $\lambda \to \infty$. A resolution of this problem has wide applications in codes for problems in which supplementary conditions at a variety of grid points are to be specified. The essence of the present development is preserved if conditions are specified at more than one point, even in the case of multidimensional grids used for approximating systems of partial differential equations (for an example, see Chapter 15). The following theorem illustrates the above mentioned limiting properties. First, denote by H_0 the subspace consisting of all members of R^{n+1} with first component zero and consider a pair of norms on this space, $N0, N1$ defined, respectively, by the Euclidean norm of R^{n+1} restricted to H_0 and the H_1. Denote by M_0 the transformation so that

$$\langle x, y\rangle_{N0} = \langle x, M_0 y\rangle_{N1},\ x, y \in H_0.$$

The transformation M_0 is induced from the spaces H_0, H_1 as in Theorem 5.4.

Theorem 8.9. *If $x \in R^{n+1}$, then*

$$\lim_{\lambda\to\infty} M_\lambda x = M_0 P x$$

for P as in (8.25).

A similar result holds where more than one point is weighted provided P is the orthogonal projection onto the subspace of R^{n+1} consisting of all grid points which are zero at the corresponding weighted grid points.

In place of a proof of Theorem 8.9 an exercise is offered. It is likely that anyone proving this theorem would want to do an exercise as follows and, in addition, if anyone does the exercise, then they would see the truth of the theorem. A key idea is to start with (8.25). To understand M_λ, let $\nu = \lambda - 1$ and consider Cramer's rule applied to $(\nu P + I)D^t D$. Cramer's rule for a square matrix has two parts: The first part is to calculate the determinant of the matrix, the second part is to construct the relevant matrix of minors of the original matrix. Sort the terms of both of these according to whether or not a term contains ν. Then observe the limiting result in Theorem 8.9. What happens is that M_0 appears as the matrix M_1 with both the first row and the first column of M_1 replaced by zeros. The corresponding result for two weighted points would be to replace, in M_1, both rows and columns corresponding to the two weighted grid points. Proceed in a similar way for more than two weighted points. The reader might note how this discussion is related to Section 8.7.

The practical significance of the above paragraph is this: A problem requiring a Sobolev gradient for a system of differential equations uses projections, at least implicitly. The main issue in constructing this projection is the determination of an imbedding operator, where for some relevant D is $M = (D^tD)^{(-1)}$. If such a transformation M is computed without regard to supplementary conditions, then for supplementary conditions which specify values at certain grid points, the needed transformation, say $\tilde{M}$, is obtained by deleting appropriate rows and columns from M.

8.9 An Example with Mixed Boundary Conditions

This section contains a Sobolev gradient construction for a system of two ordinary differential equations. Consider projections associated with some mixed boundary conditions given by the following pair of equations:

$$u'(t) = f(u(t), v(t)),\ v'(t) = g(u(t), v(t)),\ t \in [0, 1],$$

where $f, g : R^2 \to R$ are of class $C^{(1)}$. Let $H = H^{1,2}([0, 1])$ and define

$$\phi : H \to R$$

by

$$\phi(u, v) = (1/2) \int_0^1 ((u' - f(u, v))^2 + (v' - g(u, v))^2),\ u, v \in H.$$

Take $Du = \binom{u}{u'},\ u \in H$. Calculate:

$$\phi'(u, v)(h, k) = \int_0^1 ((u' - f(u, v))(h' - f_1(u, v)h - f_2(u, v)k) \tag{8.26}$$

$$+(v' - g(u, v))(k' - g_1(u, v)h - g_2(u, v)k)) = \langle \binom{Dh}{Dk}, \binom{r}{s} \rangle_{L_2([0,1])^4},$$

where

$$r = \begin{pmatrix} -(u' - f(u, v))f_1(u, v) - (v' - g(u, v))g_1(u, v) \\ u' - f(u, v) \end{pmatrix}$$

and

$$s = \begin{pmatrix} -(u' - f(u,v))f_2(u,v) - (v' - g(u,v))g_2(u,v) \\ v' - g(u,v) \end{pmatrix},$$

$u, v, h, k \in H$. Thus from (8.26),

$$\phi'(u,v)(h,k) = \langle \left(\begin{smallmatrix} Dh \\ Dk \end{smallmatrix}\right), \left(\begin{smallmatrix} Pr \\ Ps \end{smallmatrix}\right) \rangle_{L_2([0,1])^4} \tag{8.27}$$

where P is the orthogonal projection of $L_2([0,1])^2$ onto

$$\{\left(\begin{smallmatrix} u \\ u' \end{smallmatrix}\right) : u \in H\}.$$

Hence

$$(\nabla\phi)(u,v) = \left(\begin{smallmatrix} \pi Pr \\ \pi Ps \end{smallmatrix}\right),$$

where $\pi\left(\begin{smallmatrix} \alpha \\ \beta \end{smallmatrix}\right) = \alpha$, $\alpha, \beta \in H$.

Now incorporate boundary conditions, say

$$u(0) = 1, v(1) = 1.$$

Then in (8.26),

$$h \in H_1 = \{\alpha \in H : \alpha(0) = 0\},$$
$$k \in H_2 = \{\beta \in H : \beta(1) = 0\},$$

and instead of (8.27),

$$\phi'(u,v)(h,k) = \langle \left(\begin{smallmatrix} Dh \\ Dk \end{smallmatrix}\right), \left(\begin{smallmatrix} P_0 r \\ Q_0 s \end{smallmatrix}\right) \rangle_{L_2([0,1])^4} \tag{8.28}$$

where here P_0 is the orthogonal projection of $L_2([0,1])^2$ onto

$$\{D\alpha : \alpha \in H_1\}.$$

and Q_0 is the orthogonal projection of $L_2([0,1])^2$ onto

$$\{D\beta : \beta \in H_2\}.$$

Hence for these boundary conditions there is the Sobolev gradient

$$(\nabla\phi)(u,v) = \left(\begin{smallmatrix} \pi P_0 r \\ \pi Q_0 s \end{smallmatrix}\right).$$

For mixed boundary conditions, say $u(0) = v(1)$, $u(1) = 2v(0)$, there is in place of (8.28),

$$\phi'(u,v)(h,k) = P_1\left(\begin{smallmatrix} r \\ s \end{smallmatrix}\right)$$

where here P_1 is the orthogonal projection of $L_2([0,1])^4$ onto

$$\{\binom{D\alpha}{D\beta} : \alpha(0) - \beta(1) = 0, \alpha(1) - 2\beta(0) = 0,\ \alpha, \beta \in H\}.$$

Hence in this case there is the Sobolev gradient

$$(\nabla\phi)(u, v) = \pi P_1\binom{r}{s}$$

where here $\pi(\alpha, \beta, \gamma, \delta) = (\alpha, \gamma)$.

In this latter case the boundary conditions are coupled between the two components of the solution and a single orthogonal projection on $L_2([0,1])^4$ is to be calculated rather than two individual projections on $L_2([0,1])^2$. Chapter 10 contains information about construction of such projections.

Chapter 9
Continuous Newton's Method

9.1 Riemannian Metrics and a Nash-Moser Inverse Function Result

In this chapter it is shown how a Newton vector field arises from a Riemannian metric in the context of Soboles gradients. A new form of continuous Newton's method is derived and it is seen how a version of a Nash-Moser inverse function theorem comes from this form.

For motivation, suppose F is a C^2 function from a finite dimensional inner product space H to itself and denote by $\phi : H \to R$ the function so that

$$\phi(x) = \frac{1}{2}\|F(x)\|_H^2,\ x \in H. \tag{9.1}$$

Suppose in addition that $F'(x)^{-1}$ exists for all $x \in H$. For each $x \in H$ define the inner product $\langle \cdot, \cdot \rangle_x$ by

$$\langle g, h \rangle_x = \langle F'(x)g, F'(x)h \rangle_H,\ g, h \in H. \tag{9.2}$$

The space H with this family of metrics becomes a Riemannian manifold. Consider the vector field induced by ϕ on this manifold. For $x \in H$, represent the linear function $\phi'(x)$ in terms of the inner product $\langle \cdot, \cdot \rangle_x$ to get

$$\phi'(x)h = \langle h, (\nabla_x \phi)(x) \rangle_x = \langle F'(x)h, F'(x)(\nabla_x \phi)(x) \rangle_H,\ h \in H. \tag{9.3}$$

But also

$$\phi'(x)h = \langle F'(x)h, F(x) \rangle_H,\ h \in H, \tag{9.4}$$

so putting (9.3),(9.4) together one has that

$$F'(x)(\nabla_x \phi)(x) = F(x),\ x \in H,$$

i.e,

$$(\nabla_x \phi)(x) = F'(x)^{-1} F(x),$$

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_9,

the Newton vector field for F at x. Thus the Sobolev gradient of ϕ taken with respect to the Riemannian metric induced by F is the Newton vector field for F. It will be seen that this particular Sobolev gradient has some remarkable properties.

Suppose that for $x \in H$, continuous steepest descent associated with the above Newton vector field has existence on all of $[0, \infty)$, i.e., there is a unique z on $[0, \infty)$ so that

$$z(0) = x, \ z'(t) = -(\nabla_{z(t)}\phi)(z(t) = -F'(z(t))^{-1}F(z(t)), \ t \geq 0. \tag{9.5}$$

Hence

$$F'(z(t))z'(t) = -F(z(t)), \ t \geq 0$$

and therefore

$$(F(z))'(t) = -F(z(t)), \ t \geq 0.$$

From this it follows that

$$F(z(t)) = \exp(-t)F(x), \ t \geq 0 \tag{9.6}$$

since $z(0) = x$. Substituting from (9.6) into (9.5) yields

$$z(0) = x, \ z'(t) = -\exp(-t)F'(z(t))^{-1}F(x) \ t \geq 0.$$

Rescaling 'time' to $[0, 1)$ from $[0, \infty)$ this becomes

$$z(0) = x, \ z'(t) = -F'(z(t))^{-1}F(x), \ t \in [0, 1). \tag{9.7}$$

Thus

$$(F(z))'(t) = -F(x), \ t \in [0, 1),$$

and so

$$F(z(t)) = (1 - t)F(x), \ t \in [0, 1). \tag{9.8}$$

If the interval of existence in (9.7) can be extended to the closed interval $[0, 1]$ then one has

$$F(z(1)) = 0,$$

and so $z(1)$ is a desired zero of F.

This shows a feature of continuous Newton's method which seems to have no counterpart in various discrete Newton's methods, namely that the residuals $F(z(t))$ go straight to zero as $t \to 1$. This in turn inspired a new version of the Nash-Moser inverse function theorem in which the 'loss of derivatives' problem is avoided. The result uses a discretized version of (9.7) which is adapted to the case, needed for many applications to PDE, in which $F'(y)$ does not have an inverse but nevertheless for a given element g the equation

$$F'(y)h = g$$

may be solved for h for each element y some appropriate set. Specifically there is the following result from [166]:

Suppose that each of H, K, J is a Banach space with H compactly embedded in J in the sense that H forms a linear subspace of J and every bounded sequence $\{x_k\}_{k=1}^{\infty}$ in H has a subsequence convergent in J to a member of $x \in H$ so that

$$\|x\|_H \leq \limsup_{k \to \infty} \|x_k\|_H.$$

If $t > 0$ and $w \in H$, then $B_t(w)$ denotes the closed ball in H with radius t and center w.

Theorem 9.1. *Suppose that $F : H \to K$ is continuous as a function on J, $x_0 \in H$, $r > 0$ and that for each x in the interior of $B_r(x_0)$ there is*

$$h \in B_r(0)$$

so that

$$\lim_{t \to 0+} \frac{1}{t}[F(x + th) - F(x)] \ = \ -F(x_0).$$

Then there is $u \in B_r(x_0)$ so that

$$F(u) = 0.$$

Proof. Suppose that $\epsilon > 0$. Define

$$S = \{s \in [0,1] \ : \ \exists\, y \in B_{rs}(x) \text{ such that } \|F(y) - (1-s)F(x)\| \leq \epsilon s\}.$$

Note that S is closed, since $[0,1]$ is compact and every sequence in $B_r(x)$ has a subsequence convergent in J to an element of $B_r(x)$ (and F is continuous from J to K). Denote $\sup S$ by λ and suppose that $\lambda < 1$. Pick y in $B_{\lambda r}(x)$ for which

$$\|F(y) - (1-\lambda)F(x)\| \leq \epsilon\lambda,$$

and then choose h in $B_r(0)$ and δ in $(0, 1-\lambda]$ so that

$$\|\frac{1}{\delta}(F(y + \delta h) - F(y)) + F(x)\| \leq \epsilon,$$

that is,

$$\|(F(y + \delta h) - F(y)) + \delta F(x)\| \leq \epsilon\delta.$$

Then $\|y + \delta h\| \leq (\lambda + \delta)r$ and

$$\begin{aligned} &\|F(y + \delta h) - (1 - \delta - \lambda)F(x)\| \\ &\qquad \leq \|F(y + \delta h) - F(y) + \delta F(x)\| + \|F(y) - (1-\lambda)F(x)\| \leq \epsilon(\delta + \lambda), \end{aligned}$$

so $\delta + \lambda$ belongs to S, a contradiction. Therefore $\lambda = 1$.

Hence, for each $\epsilon > 0$ there is u_ϵ in $B_r(x)$ so that $\|F(u_\epsilon)\| \leq \epsilon$. By the continuity of F and the fact that every sequence in $B_r(x)$ has a subsequence convergent in J to a member of $B_r(x)$, there exists u in $B_r(x)$ such that $F(u) = 0$. □

This theorem implies the following version of a Nash-Moser inverse function theorem:

Theorem 9.2. *Suppose that $F : H \to K$ is continuous as a function on J, $g \in K$, $r, M > 0$, and that for each x in the interior of $B_r(0)$ there is*

$$h \in B_M(0)$$

so that

$$\lim_{t \to 0+} \frac{1}{t}[F(x+th) - F(x)] \ = \ g.$$

If $\lambda \in [0, r/M)$ there is $x \in B_{\lambda M}$ so that

$$F(x) \ = \ \lambda g.$$

9.2 Newton's Method from Optimization

The development in this section arose in an attempt to define something like a Sobolev gradient in cases where the objective function is not on a function space. The question is raised as to how effective gradients may be defined in such cases. For this turn to another criteria for defining a Sobolev gradient.. Suppose that n is a positive integer and ϕ is a $C^{(3)}$ function on R^n. Seek $\beta : R^n \times R^n \to R$, $\beta \in C^{(3)}$, so that if $x \in R^n$, the problem of finding a critical point h of

$$\phi'(x)h \text{ subject to the constraint } \quad \beta(x,h) = c \in R$$

leads us to a numerically sound gradient. What is required of β? One criterion is that the sensitivity of h in $\beta(x,h)$ should somewhat match the sensitivity of h in $\phi'(x)h$. This suggests a choice of

$$\beta(x,h) = \phi(x+h), \ x, h \in R^n.$$

For $x \in R^n$, define

$$\alpha(h) = \phi'(x)h, \gamma(h) = \beta(x,h), \ h \in R^n. \tag{9.9}$$

If h is an extremum of α subject to the constraint $\gamma(h) = c$ (for some $c \in R$), then, using Lagrange multipliers, it must be that

$$(\nabla\alpha)(h) \text{ and } (\nabla\gamma)(h) \text{ are linearly dependent.}$$

But

$$(\nabla\alpha)(h) = (\nabla\phi)(h) \text{ and } (\nabla\gamma)(h) = (\nabla\phi)(x + h).$$

Some consequences are summarized in the following:

Theorem 9.3. *Suppose that ϕ is a real-valued $C^{(3)}$ function on R^n, $x \in R^n$, and (9.9) holds. Suppose also that $((\nabla\phi)'(x))^{-1}$ exists. Then there is an open interval J containing 1 such that if $\lambda \in J$, then*

$$\lambda(\nabla\phi)(x) = (\nabla\phi)(x + h)$$

for some $h \in R^n$.

Proof. Since $((\nabla\phi)'(x))^{-1}$ exists, then $((\nabla\phi)'(y))^{-1}$ exists for all y in some region G containing x. The theorem in the preface gives that there is an open interval J containing 1 on which there is a unique function z so that

$$z(1) = 0, z'(t) = ((\nabla\phi)'(x + z(t)))^{-1}(\nabla\phi)(x)), \ t \in J.$$

This is rewritten as

$$((\nabla\phi)'(x + z(t))z'(t) = (\nabla\phi)(x), \ t \in J.$$

Take anti-derivatives to get

$$(\nabla\phi)(x + z(t)) = t(\nabla\phi)(x) + c_1, \ t \in J.$$

But $c_1 = 0$ since $z(1) = 0$ and the argument is finished. □

Note that

$$z'(1) = ((\nabla\phi)'(x))^{-1}(\nabla\phi)(x)$$

is the Newton direction of $\nabla\phi$ at x. For a given x, the sign of

$$\langle((\nabla\phi)'(x))^{-1}(\nabla\phi)(x), (\nabla\phi)(x)\rangle_{R^n}$$

is important. If this quantity is positive then

$$((\nabla\phi)'(x))^{-1}(\nabla\phi)(x)$$

is an ascent direction; if negative it is a descent direction; if zero, then x is already a critical point of ϕ.

Chapter 10
More About Finite Differences

In Chapters 2, 8 there are already Sobolev gradients in a finite dimensional settings. The present chapter illustrates additional approximations to function space problems, but it is pointed out that these finite dimensional problems themselves fit the general theory of Chapters 4,5. The present chapter might be read in connection with Chapter 8, with which there is some overlap.

10.1 Finite Differences and Sobolev Gradients

Some additional ideas about Sobolev gradients for finite dimensional problems are illustrated by two examples. The first example is a variation on (8.17). That such variations exist illustrates the idea that it is common to have a choice among competing, often equally good, differencing schemes connected with a given system of differential equations.

Example 10.1. Pick a positive integer n and

$$G = (0, 1, \ldots, n).$$

Denote by H the collection of all real-valued functions on G and take for the first norm for H a standard Euclidean norm. A second norm for H will be introduced later. Define $D : H \to R^{2n}$ by

$$Du = \begin{pmatrix} D_0 u \\ D_1 u \end{pmatrix},\ u \in H \tag{10.1}$$

where, for $\delta = \frac{1}{n}$,

$$(D_0 u)_p = \frac{1}{2}(u_p + u_{p-1})$$

and

$$(D_1 u)_p = \frac{1}{\delta}(u_p - u_{p-1}),\ p = 1, \ldots, n. \tag{10.2}$$

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_10,

Denote by $F : R^2 \to R$ a C^1 function. Consider the problem of finding a critical point of ϕ:

$$\phi(u) = \frac{1}{2}\|F(Du)\|_H^2,\ u \in H.$$

Note that for $u \in H$, $F(Du)$ is understood as

$$(F(Du))_p = F\begin{pmatrix}(D_0u)_p \\ (D_1u)_p\end{pmatrix},\ p \in G.$$

We seek a Sobolev gradient of ϕ with respect to the (second) inner product on H:

$$\langle f, g\rangle_D = \langle Df, Dg\rangle_{R^{2n}},\ f, g \in H, \tag{10.3}$$

a finite dimensional analog of the $H^{1,2}([0,1])$.

Take a Fréchet derivative:

$$\phi'(u)h = \langle F'(Du)Dh, F(Du)\rangle_H = \langle Dh, F'(Du)^t F(Du)\rangle_{R^{2n}}, \tag{10.4}$$
$$= \langle h, D^t F'(Du)^t F(Du)\rangle_H\ u, h \in H, \tag{10.5}$$

Accordingly,

$$(\nabla_0\phi)(u) = D^t F'(Du)^t F(Du) \tag{10.6}$$

where $\nabla\phi$ is the ordinary gradient of ϕ.

Alternatively, from (10.4),

$$\phi'(u)h = \langle F'(Du)Dh, F(Du)\rangle_{R^{2n}} \tag{10.7}$$
$$= \langle Dh, PF'(Du)^t F(Du)\rangle_{R^{2n}},\ u, h \in H, \tag{10.8}$$

where P is the orthogonal projection of R^{2n} onto

$$\{\begin{pmatrix}D_0u \\ D_1u\end{pmatrix} : u \in H\}.$$

Note that

$$P = D(D^tD)^{-1}D^t.$$

since $D(D^tD)^{-1}D^t$ is symmetric, its range is a subset of the range of D, it is idempotent and is fixed on the range of D. Hence from (10.7)

$$\begin{aligned}\phi'(u)h &= \langle Dh, D(D^tD)^{-1}D^tF'(Du)^t F(Du)\rangle_{R^{2n}}, \\ &= \langle h, (D^tD)^{-1}D^tF'(Du)F(Du)\rangle_D \\ &= \langle h, (D^tD)^{-1}(\nabla_0\phi)(u)\rangle_D,\ u, h \in H.\end{aligned}$$

Thus the Sobolev gradient $\nabla_D\phi$ of ϕ at the element $u \in H$, with respect to the inner product (10.3) is given by

$$(\nabla_D \phi)(u) = (D^t D)^{-1}(\nabla_0 \phi)(u),\ u \in H,$$

the gradient sought.

Example 10.2. A second example is for a two dimensional domain. Suppose n is a positive integer and

$$G = \{(i,j) : i,j \in (0,1,\ldots,n)\} \tag{10.9}$$

and H the collection of all real-valued functions on G. Define $D : H \to R^{3n}$ by

$$Du = \begin{pmatrix} D_0 u \\ D_1 u \\ D_2 u \end{pmatrix} \tag{10.10}$$

where

$$(D_0 u)_{i,j} = \frac{(u_{i,j} + u_{i-1,j}) + (u_{i,j-1} + u_{i-1,j-1})}{2\delta}, \tag{10.11}$$

$$(D_1 u)_{i,j} = \frac{(u_{i,j} - u_{i-1,j}) + (u_{i,j-1} - u_{i-1,j-1})}{2\delta},$$

$$(D_2 u)_{i,j} = \frac{(u_{i,j} - u_{i,j-1}) + (u_{i-1,j} - u_{i-1,j-1})}{2\delta},\ i,j = 1,\ldots,n.$$

Note that $D : H \to R^N$ where $N = 3n^2$, the total number of components in (10.10). Take the standard Euclidean norm for the first norm of H. Suppose that

$$F : R^3 \to R$$

is a C^1 function. Consider the problem of finding a critical point of ϕ where

$$\phi(u) = \frac{1}{2}\|F(Du)\|_H^2. \tag{10.12}$$

In (10.12), $F(Du) : H \to H,\ u \in H$ is understood as

$$(F(Du))_{i,j} = F\begin{pmatrix} (D_0 u)_{i,j} \\ (D_1 u)_{i,j} \\ (D_2 u)_{i,j} \end{pmatrix}$$

As in the first example the ordinary gradient $\nabla_0 \phi$ of ϕ is

$$(\nabla_0 \phi)(u) = D^t (F'(Du))^t F(Du),\ u \in H.$$

Note that the bilinear function $\langle \cdot,\cdot \rangle_D$ defined by

$$\langle f,g \rangle_D = \langle Df, Dg \rangle_{R^N},\ f,g \in H,$$

is not positive definite since for

$$f_{i,j} = (-1)^{i+j},\ i, j = 0, 1, \ldots, n,$$

$Df = 0$. As a remedy to this lack of positive definiteness, use instead a closely related inner product. This is a two dimensional version of a device already used in Chapter 8. Define

$$E : H \to R^K, K = R^{(n+1)^2+2n},$$

so that if $u \in H$, then

$$Eu = \begin{pmatrix} u \\ D_1 u \\ D_2 u \end{pmatrix}. \tag{10.13}$$

Define

$$\langle f, g \rangle_E = \langle Ef, Eg \rangle_{R^K},\ f, g \in H.$$

Then

$$\begin{aligned}(\phi'(u))h &= \langle F'(Du)Dh, F(Du)\rangle_H = \langle h, (\nabla_0\phi)(u)\rangle_H \\ &= \langle h, (E^tE)(E^tE)^{-1}(\nabla_0\phi)(u)\rangle_H = \langle Eh, E(E^tE)^{-1}(\nabla_0\phi)(u)\rangle_{R^K} \\ &= \langle h, (E^tE)^{-1}(\nabla_0\phi)(u)\rangle_E, u, h \in H.\end{aligned}$$

Thus the Soboelv gradient sought is given by

$$(\nabla_E\phi)(u) = (E^tE)^{-1}(\nabla_0\phi)(u),\ u \in H. \tag{10.14}$$

A generalization is straightforward to the case in which members of H take values in some Euclidean space of dimension more than one. The development leading to (10.14) indicates that the transformation D used in defining a finite difference version of a system of partial differential equations need not be precisely the same as an embedding operator that is used to transform the ordinary gradient into a Sobolev gradient. In the present case, D is a convenient central difference operator for which D^tD does not have an inverse. The transformation E is closely related to D but E^tE *does* have an inverse.

10.2 Supplementary Conditions Again

Equations (8.3) and (5.6) deal with boundary or supplementary conditions and Sobolev gradients. Here the subject arises again in a somewhat different form. In (8.3) a Sobolev gradient for a linearly constrained problem was constructed in two steps: First a Sobolev gradient, which did not take into account supplementary conditions, was constructed. Then this gradient was projected to yield a Sobolev gradient that did take account of supplementary conditions. In the present section it is indicated how to combine these two steps, potentially both a coding and a computational time saver.

Here is a more efficient computational scheme. Denote by H_0 a subspace of H. Use both D and E in Example 10.2 as well as the inner product $\langle \cdot, \cdot \rangle_D$ and the function F. Denote by π_0 the orthogonal projection of H onto H_0. Denote by D_r, E_r ('r' for 'restricted') the restrictions of D, E, respectively to H_0. What is D_r^t?

Lemma 10.3.

D_r^t is the restriction of $\pi_0 D$ to H_0.

Proof. Suppose $g, h \in H_0$. Then

$$\begin{aligned}\langle D_r g, h\rangle_{H_0} &= \langle Dg, h\rangle_H = \langle g, D^t h\rangle_H \\ &= \langle \pi_0 g, D^t h\rangle_H = \langle g, \pi_0 D^t h\rangle_H = \langle g, \pi_0 D^t h\rangle_{H_0},\end{aligned}$$

□

so

$$D_r^t h = \pi_0 D^t h.$$

Here D_r^t is used as adjoint of D_r relative to the space H_0, not as the transpose of a matrix. It is hoped that a reader is by now comfortable with using different adjoints for a single transformation. This situation is worse in Section 8.8, where there is a continuum of adjoints for some linear transformations. Similar comments hold for E_r.

Pick $w \in H$ and define $\alpha : H_0 \to R$ by

$$\alpha(x) = \phi(w + x),\ x \in H_0.$$

An expression for $\nabla\alpha$ is sought relative to the inner product $\langle \cdot, \cdot \rangle_D$ restricted to H_0. Note that $(E_r^t E_r)^{-1}$ exists since $E_r^t E_r$ is the dilation of the invertible transformation $E^t E$ to H_0.

Theorem 10.4.

$$(\nabla\alpha)(x) = (E_r^t E_r)^{-1}\pi_0((\nabla_0\phi)(x + w)),\ x \in H_0.$$

is the gradient of α at x with respect to the H_D metric, $\nabla_0\phi$ being the ordinary gradient of ϕ.

Proof. Suppose $x, h \in H_0$. Then

$$\begin{aligned}\alpha'(x)h &= \phi'(w + x)h = \langle h, (\nabla_0\phi)(w + x)\rangle_H \\ &= \langle \pi_0 h, (\nabla_0\phi)(w + x)\rangle_{H_0} = \langle h, \pi_0(\nabla_0\phi)(w + x)\rangle_{H_0}.\end{aligned}$$

Note further that for $x, h \in H_0$,

$$\begin{aligned}\alpha'(x)h &= \langle h, (E_r^t E_r)(E_r^t E_r)^{-1}(\nabla_0\phi)(w+x)\rangle_H \\ &= \langle E_r h, E_r(E_r^t E_r)^{-1}(\nabla_0\phi)(w+x)\rangle_{R^K} \\ &= \langle h, (E_r^t E_r)^{-1}(\nabla_0\phi)(w+x)\rangle_D.\end{aligned}$$

□

In (8.11) a Sobolev gradient $(\nabla\phi)(w+z)$ was first computed. This was followed by P_Q. The work in each of these steps is roughly the same. In the present section, only one linear system is solved, i.e., to calculate the effect of $(E_r^t E_r)^{-1}$.

A word on these inverses which are generally present in all Sobolev gradient constructions connected with problems in differential equations. It would be unusual to actually calculate an inverse. For problems with a high number of gridpoints (for three dimensional grids, often $10^6 = 100^3$ points is minimal). Generally, $D^t D$ is sparse, but its inverse, if it has one, is full, so that in the case of a three dimensional grid with 100 gridpoints on each side of a cubical region, a full matrix would have 10^{12} entries, a serious computing problem. Reasonable alternatives include the following:

- Use MatLab to solve linear systems. Generally the sparse matrix solvers are excellent.
- Use an iterative method such as Jacobi's method or Gauss-Seidel iteration.
- Many cases in which a grid has constant mesh size in each direction parallel to an axis, eigenvalues and eigenvectors of a relevant laplacian are known. In this case the relevant $D^t D$ may be put in diagonal form with respect to a basis of eigenvectors of some version of a laplacian are known and consequently the action of the needed inverse can be easily calculated. (See for example Chapter 27).
- Use of one of many excellent packages: Fast Poisson Solvers, for example.

10.3 Graphs and Sobolev Gradients

For our purposes, a graph is a finite collection G with n elements for some integer $n > 2$, together with a collection E each element of which is an ordered pair of elements of G (an edge). Why include considerations about graphs in the present volume? First given any grid on which a system of partial differential equations is differenced, there is a corresponding graph, the nodes of which are the grid points and the edges are intervals going between adjacent nodes in the differencing. Some problems based on fractal domains have natural graph theoretic formulations (See for example Chapter 27). To each element q of E there is a unique positive number w_q, called the weight of q.

It is required that G be connected in the sense that for each two elements c, d of G, there is a sequence $q_1, \ldots, q_m$ of edges so that each two consecutive members of this sequence have precisely one term in common and so the first and last terms of this sequence contain c and d respectively. Denote by $C(G), C(E)$ the collection of real valued functions on G, E respectively. In the language of graph theory, this structure would be called a connected, weighted, directed graph.

Define the difference transformation D with domain $C(G)$ so that if $q = (a, b) \in E$ and $f \in C(G)$, then

$$(Df)(q) = \frac{f(b) - f(a)}{w_q}$$

where q is the ordered pair (a, b). Note that the range of D is in $C(E)$.

Define the graph laplacian L for G by

$$L = D^t D,$$

the above transpose taken with respect to the standard inner products on $C(G), C(E)$ respectively. If $w_q = 1$ for all $q \in E$, L is the standard graph laplacian (cf. [44]). Note that L does not depend on the particular orientation chosen. If, for example, one of the ordered pairs $(a, b) \in E$ is replaced by (b, a), the definition of D changes but $D^t D$ does not.

If Ω is a rectangle and G is a rectangular grid on Ω which partitions Ω into squares with sides of length δ, then it is an exercise, worth doing, to see that the corresponding laplacian L is just a differenced version of the Neumann laplacian.

A class of particularly interesting graphs can be generated by the following. Denote by M a compact connected Riemannian manifold which has charts $\phi_1, \ldots, \phi_N$ whose domains cover M and suppose that these charts all have range $[0, 1]^2$. Take a square grid G_0 of $[0, 1]^2$ and define

$$G = \bigcup_{i=1,\ldots,N} \{\phi_i^{-1} G_0\}.$$

Weight each edge of E for G by the distance, in the sense of Riemannian geometry, between its two endpoints (pick any orientation for G). Depending on how the distances are chosen and how fine a mesh is chosen for G_0, graphs G seem to emulate any compact, connected Riemannian manifold. The spectrum of a corresponding laplacian L is of interest. Eigenvalues and eigenvectors of L can be easily calculated by a MatLab code. The inverse of $I + D^t D$ is a transformation M as in Theorem 5.4.

It is not necessary in the above to have each pair of points in G connected by an edge. Computations indicate that for two relatively distant points of G, the resulting inverse of laplacian is quite insensitive to whether the corresponding edge is included or not.

10.4 Digression on Adjoints of Difference Operators

We pause here to indicate an example of a rather general phenomenon which occurs when one emulates a differential operator with a difference operator. Consider for an $n \times (n+1)$ matrix for D_1 as indicated in (10.2). The transpose of D_1 is then denoted by

$$D_1^t. \tag{10.15}$$

Commonly the derivative operator (call it L here to not confuse it with D) on $L_2([0,1])$ is taken to have domain those points in $L_2([0,1])$ which are also in $H^{1,2}([0,1])$. Denoting by L^t the adjoint of L (considered as a closed densely defined unbounded operator on $L_2([0,1])$), (as has been already noted in several places in this work) that the domain of L^t is

$$\{u \in H^{1,2}([0,1]) : u(0) = 0 = u(1)\}. \tag{10.16}$$

Furthermore,

$$L^t u = -u', u \text{ in the domain of } L^t.$$

From (10.15), if $v = (v_0, v_1, ..., v_n) \in R^{n+1}$,

$$D_1^t v = (\frac{-v_1}{\delta}, \frac{-(v_2 - v_1)}{\delta}, ..., \frac{-(v_n - v_{n-1})}{\delta}, \frac{v_n}{\delta}) \tag{10.17}$$

so that D_1^t on R^n is like $-D_1$ would be on R^n except for the first and last terms of (10.17). Remember that $\delta = 1/n$. As $n \to \infty$, the condition $u(0) = 0 = u(1)$ in (10.16) is forced by the presence of the succession of first and last terms of the rhs of (10.17). It would be possible to develop the subject of boundary conditions for adjoints of differential operators (particularly as to exactly what is to be in the domain of the adjoint - the formal expression for an adjoint is usually clear) by means of limits of difference operators on finite dimensional emulations of $L_2(\Omega), \Omega \subset R^m$ for some positive integer m. This is written knowing that these adjoints are rather well understood. Nevertheless it seems that it might be of interest to see domains of adjoints obtained by something like the above considerations. See [229] for the function space to which the above relates.

10.5 A First Order Partial Differential Equation

Next an example is given which shows how a finite difference approximation for a partial differential equation fits our scheme. A differencing scheme is used that is different from the one in Example 10.2.

Example 10.5. Suppose n is a positive integer and G is the grid composed of the points

$$\{(i/n, j/n)\}_{i,j=0}^{n}.$$

Denote by G_d the subgrid

$$\{(i/n, j/n)\}_{i,j=1}^{n-1}.$$

Denote by H the $(n+1)^2$ dimensional space whose points are the real-valued functions on G and denote by H_d the $(n-1)^2$ dimensional space whose points are the real-valued functions on G_d. Denote by D_1, D_2 the functions from H to H_d so that if $u \in H$, then

$$D_1 u = \{\frac{u_{i+1,j} - u_{i-1,j}}{2\delta}\}_{i,j=1}^{n-1}$$

and

$$D_2 u = \{\frac{u_{i,j+1} - u_{i,j-1}}{2\delta}\}_{i,j=1,n}^{n-1}.$$

Denote by D the transformation from H to $H \times H_d \times H_d$ so that

$$Du = \begin{pmatrix} u \\ D_1 u \\ D_2 u) \end{pmatrix} u \in H.$$

For an example, define $F : R^3 \to R$ so that

$$F(r, s, t) = s + rt,\ (r, s, t) \in R^3.$$

Then the problem of finding $u \in H$ such that

$$F(Du) = 0$$

is a problem of finding a finite difference approximation to a solution z to the viscosity free Burgers' equation:

$$z_1 + z z_2 = 0 \tag{10.18}$$

on $[0, 1] \times [0, 1]$. For a metric on H choose the following finite difference analogue of the norm on $H^{1,2}([0, 1] \times [0, 1]$, namely,

$$\|u\|_D = (\|u\|^2 + \|D_1 u\|^2 + \|D_2 u\|^2)^{1/2},\ u \in H, \tag{10.19}$$

All norms and inner products without subscripts in this example are Euclidean. Define then ϕ with domain H so that

$$\phi(u) = \|F(Du)\|^2/2, u \in H.$$

Compute (with $\pi = D^{-1}$))

$$\begin{aligned}\phi'(u)h &= \langle F'(Du)Dh, F(Du)\rangle \\ &= \langle Dh, (F'(Du))^t F(Du)\rangle = \langle Dh, PF'(Du)^t F(Du)\rangle \\ &= \langle h, \pi PF'(Du)^t F(Du)\rangle_D = \langle h, (D^tD)^{-1}D^tF'(Du)^tF(Du)\rangle_D\end{aligned}$$

so that

$$(\nabla_D\phi)(u) = (D^tD)^{-1}D^tF'(Du)^tF(Du) = (D^tD)^{-1}(\nabla\phi)(u)$$

where $\langle\ ,\ \rangle_D$ the inner product associated with $\|\ \ \|_D$ (the preceding use the facts that $P = D(D^tD)^{-1}D)$ and $(\nabla\phi)(u)$ is the ordinary gradient of ϕ, $u \in H$). A gradient which takes into account boundary conditions may be introduced into the present setting much as in Examples 2 and 3. Pause here to recall briefly some known facts about (10.18).

Theorem 10.6. *Suppose z is a C^1 solution on $\Omega = [0,1]\times[0,1]$ to (10.18). Then $[0,1]\times[0,1]$ is the union of a collection Q of closed intervals such that*
(i) no two members of Q intersect,
(ii) if $J \in Q$, then each end point of J is in $\partial\Omega$,
(iii) if $J \in Q$ and J is nondegenerate, then the slope m of J is such that

$$m = z(x),\ x \in J.$$

Members of Q are characteristic lines for (10.18). Some reflection reveals that no nondegenerate interval S contained in $\partial\Omega$ is small enough so that if arbitrary smooth data is specified on S then there would be a solution z to (10.18) assuming that data on S. This is another instance of the fundamental fact that for many systems of nonlinear partial differential equations the set of all solutions on a given region is not conveniently specified by means of conditions on some designated boundary. This writer did numerical experiments in 1976–77 (unpublished) using a relative of a Sobolev gradient (10.18) (the name 'Sobolev gradient' was not invented yet). It was attractive to have a numerical method which was not boundary condition dependent. It was noted that a limiting function from a steepest descent process had a striking resemblance to the starting function used (recall that for linear homogeneous problems the limiting value is the nearest solution to the starting value). It was then that the idea of a foliation emerged: the relevant function space is divided into leaves in such a way that two functions are in the same leaf provided they lead (via steepest descent) to the same solution. It still remains a research problem to characterize such foliations even in problems such as (10.18). See Chapters 19, 20 in connection with corresponding foliations. More specifically

$$r, s \in H = H^{1,2}(\Omega)$$

are equivalent provided that if

$$z_r(0) = r,\ z_s(0) = s,$$

and

$$z_r'(t) = -(\nabla\phi)(z_r(t)), z_s'(t) = -(\nabla\phi)(z_s(t)),\ t \geq 0, \tag{10.20}$$

then

$$\lim_{t\to\infty} z_r(t) = \lim_{t\to\infty} z_s(t),$$

where

$$\phi(u) = \frac{1}{2}\int_{\Omega}(u_1 + uu_2)^2,\ u \in H.$$

It would be good to understand the topological, geometrical and algebraic nature of these equivalence classes. Each contains exactly one solution to (10.18). The family of these equivalence classes should characterize the set of all solutions to (10.18) and provide a point of departure for further study of this equation. The gradient in (10.20) is the function $\nabla\phi$ so that if $u \in H$, then

$$\phi'(u)h = \langle h, (\nabla\phi)(u)\rangle_H,\ h \in H.$$

Chapter 8 deals with supplementary conditions generally. Specifically, chapters 19, 20 deal rather generally with foliations which arise as in the above. This example influenced this writer's work considerably and the problem of coding this problem is often suggested to students.

10.6 A Second Order Partial Differential Equation

Here now is an example of a Sobolev gradient for numerical approximations to a second order problem. Following are alternative ways to treat a second order problem.

- If a second order problem is an Euler equation for a first order variational principle, one may deal with the underlying problem using only first order derivatives as will be indicated in Chapter 11.
- In any case a problem can always be converted from a second order problem into a system of first order equations by introducing one or more unknowns. Frequently there are several ways to accomplish this.

Example 10.7. In any case, if one is determined to treat a second order problem directly, one may proceed as follows. Suppose that

$$\Omega = [0,1]\times[0,1]$$

and that our second order problem is Laplace's equation on Ω. The following is not partcularly recommended for coding; it is for purposes of illustration only.

Take a rectangular grid and take H to be the vector space of all real-valued functions on this grid. Define D_0, D_1, D_2 on H as in the preceding section. Fpr second difference operators, take

$$(D_{11}u)_{i,j} = \frac{(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})}{\delta^2}$$
$$(D_{12}u)_{i,j} = \frac{(u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1})}{\delta^2},$$

$$(D_{22}u)_{i,j} = \frac{(u_{i,j+1} - 2u_{i,j} + u_{i,j-1})}{\delta^2},\ i,j = 1,2,...,n-1.$$

Define:

$$Du = (D_0u, D_1u, D_2u, D_{11}u, D_{12}u, D_{22}u),\ u \in H,$$

and take, for $u \in H$, $\|u\|_D^2 =$

$$\|D_0u\|^2+\|D_0u\|^2+\|D_1u\|^2+\|D_2u\|^2+\|D_{11}u\|^2+\|D_{12}u\|^2+\|D_{22}u\|^2, \quad (10.21)$$

emulating the $H^{2,2}(\Omega)$ norm. Define ϕ on H so that

$$\phi(u) = \frac{1}{2}\sum_{i,j=1}^{n-1}((D_{11}u)_{i,j} + (D_{22}u)_{i,j})^2,\ u \in H.$$

Thus if $u, h \in H$,

$$\phi'(u)h = \sum_{i,j=1}^{n-1}((D_{11}u)_{i,j}(D_{11}h)_{i,j} + (D_{22}u)_{i,j}(D_{22}h)_{i,j})$$

and so

$$\begin{aligned}\phi'(u)h &= \langle Dh, (0,0,0,D_{11}u,0,D_{11}u)\rangle \\ &= \langle Dh, P(0,0,0,D_{11}u,0,D_{22}u)\rangle \\ &= \langle h, \pi P(0,0,0,D_{11}u,0,D_{11}u)\rangle_D\end{aligned}$$

and so

$$(\nabla_D\phi)(u) = \pi P(0,0,0,D_{11}u,0,D_{11}u)$$

where $\langle\ ,\ \rangle_D$ denotes the inner product derived from (10.21) and P is the orthogonal projection of H^6 onto $R(D)$. In this particular case, of course, the work involved in constructing P is at least as much as that of solving Laplace's equation directly.

In [189], there is described a computer code which solves a general second order quasi-linear partial differential equation on an arbitrary grid whose intervals are parallel to the axes of R^2. If boundary conditions on $\partial\Omega$ are required, then the above constructions are modified along the lines of Chapter 10. The various vectors h appearing above are to be in

$$H_0 = \{u \in H : u_{i,j} = 0 \text{ if one of } i \text{ or } j = 0 \text{ or } n\}.$$

Then the resulting gradient $\nabla_D \phi$ will have range in H_0. It is written in terms of P_0, the orthogonal projection of H_0^6 onto $R(D)$.

In Chapter 27 there is an extensive discussion of the use of the numerical of eigenvalues in efficient calculations in Sobolev gradient problems.

Chapter 11
Sobolev Gradients for Variational Problems

Many problems in partial differential equations are cast as critical point problems for real valued functions. This chapter indicates how Sobolev gradients relate to such problems. Problems in a number of chapters to follow are cast in terms of variational principles.

Suppose each of m, n is a positive integer, Ω is a region in R^n, $F : R^{n+1} \to R$ a C^1 function and $\phi : H = H^{m,2}(\Omega) \to R$ so that ϕ with

$$\phi(u) = \int_\Omega F(Du),\ u \in H \tag{11.1}$$

is also a C^1 function, where Du is a list starting with u and following with partial derivatives of u up to order m, Actually, m is chosen minimally so that ϕ is C^1 and the integrand in

$$\phi'(u)h = \int_\Omega F'(Du)Dh, \tag{11.2}$$

is in $L_1(\Omega),\ u, h \in H$.

11.1 Minimizing Sequences

Supposing that ϕ is bounded from below, a common way to try to find a critical point of (11.1) is to pick a minimizing sequence for ϕ, that is, a sequence

$$\{u^k\}_{k=1}^\infty$$

so that

$$\lim_{k\to\infty} \phi(u^k) = \inf_{u\in H} \phi(u)$$

in the hope that some subsequence can be shown to converge to $u \in H$ which is a critical point of ϕ (cf. [59]). This procedure produces a critical point in many important instances but it is clear that such a process is

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not constructive. Even successfully applied, the process yields little information about a critical point u. It is an aim of the present volume to produce constructive existence arguments which are naturally tied to corresponding numerical methods as is indicated in the next section.

11.2 Euler-Lagrange Equations

A second attack on finding a critical point of (11.1) is through a corresponding Euler-Lagrange equation. For simplicity, suppose $m = 1$ and let

$$Du = \begin{pmatrix} u \\ \nabla u \end{pmatrix}.$$

Then (11.2) may be rewritten:

$$\phi'(u)h = \langle (Dh, (\nabla F)(Du)\rangle_{L_2(\Omega)^3},\ u, h \in H. \tag{11.3}$$

What amounts to an integration by parts (assuming existence of the needed second derivatives) gives

$$\phi'(u)h = \langle h, D^t(\nabla F)(Du)\rangle_{L_2(\Omega)} + \text{ boundary terms},\ u, h \in H. \tag{11.4}$$

If for some $u \in H$ one has $\phi'(u)h = 0$ for all $h \in H$, it holds that some combination of values and derivatives of u on the boundary of Ω be zero and also the corresponding Euler-Lagrange equation

$$D^t(\nabla F)(Du) = 0$$

hold. Now it is common that at a critical point u of ϕ the necessary second derivatives do exist, but the requirement that the boundary terms be zero for all $h \in H$ imposes often nonlinear boundary conditions on u ('natural boundary conditions', as for example Chapter 14). One might be able to solve this Euler-Lagrange system under these natural boundary conditions but there is certainly no general procedure for doing so.

11.3 Sobolev Gradient Approach

Sobolev gradients provide a constructive approach to such problems. Just before the step (11.4), note that (11.3) gives

$$\phi'(u)h = \langle Dh, P(\nabla F)(Du)\rangle_{\text{Ł}_2(\Omega)^3},\ u, h \in H$$

where P is the orthogonal projection of $L_2(\Omega)^3$ onto

$$\{\begin{pmatrix} u \\ \nabla u \end{pmatrix} : u \in H\}.$$

Hence with

$$\pi\begin{pmatrix} u \\ w \end{pmatrix} = u,\ u \in H, w \in L_2(\Omega)^2,$$

one has

$$\phi'(u)h = \langle h, \pi P((\nabla F)(Du))\rangle_H,\ u, h \in H.$$

Thus the Sobolev gradient $(\nabla_S \phi)(u)$ of ϕ relative to the norm H is given by

$$(\nabla_S \phi)(u) = \pi P((\nabla F)(Du)),\ u \in H.$$

If Dirichlet boundary condtions are to be imposed on critical points of (11.2), then the projection P above would be onto

$$\{\begin{pmatrix} u \\ \nabla u \end{pmatrix} : u \in H, u = 0 \text{ on } \partial\Omega\}.$$

Other boundary conditions can be imposed as indicated in Chapter 8. Note that 'boundary conditions', better said 'supplementary conditions' can be imposed just as easily on an arc interior to Ω, for example. This observation opens up a much broader class of supplementary conditions than is conventionally possible to treat. In any case with gradients constructed as in this section, a critical point may be sought using some of the results of Chapter 4 by means of solutions z to

$$z(0) = x \in H,\ z'(t) = -(\nabla_S \phi)(z(t)),\ t \geq 0. \tag{11.5}$$

Now in cases where ϕ is specified as

$$\phi(u) = \frac{1}{2}\|G(u)\|_K^2, u \in H,$$

for some function $G : H \to K$, K being a second Hilbert space, one might want a zero of F, not just a critical point of ϕ, but results of Chapter 4 indicate that often a critical point of ϕ is also a zero of F.

In case a critical point of ϕ might be unstable (as suggested, perhaps by numerical computations) one may try to use results of Chapter 4 applied to a second functional J :

$$J(u) = \frac{1}{2}\|(\nabla\phi)(u)\|_H^2,\ u \in H.$$

Then any zero of J is a critical point of ϕ and such a zero of J is likely to be stable. Here are some details on how this works out:

First note that

$$\begin{aligned} J'(u)h &= \langle (\nabla\phi)'(u)h, (\nabla\phi)(u)\rangle_H \\ &= \langle h, (\nabla\phi)'(u)(\nabla\phi)(u)\rangle_H,\ u,h \in H \end{aligned}$$

since $(\nabla\phi)'(u)$ is symmetric due to the fact that ϕ is C^2. Hence

$$(\nabla J)(u) = (\nabla\phi)'(u)(\nabla\phi)(u),\ u \in H. \tag{11.6}$$

For small enough $\delta > 0$, the gradient in 11.6 is well approximated by

$$\frac{1}{\delta}[(\nabla\phi)(u + \delta(\nabla\phi)(u)) - (\nabla\phi)(u)].$$

Thus if one has a routine in place for calculating a Sobolev gradient of ϕ, the same routine may be used a second time to get a useable approximation to the Sobolev gradient of J. This has been particularly useful in cases in which unstable critical points of functionals are being sought. Numerical steepest descent for ϕ sometimes tends to slide by a critical point of ϕ whereas steepest descent for J converges nicely to a critical point of ϕ.

In a general case, one must take care that a m in (11.1) be chosen so that (11.1), (11.2) are properly defined. The dimension of the space and the nature of the nonlinearities are, of course, crucial in these cases (see [2, 59]). Generally, the choice of m determines the number of derivatives that need to be include in the relevant operator D.

To reiterate, (11.5) is an ordinary differential equation, albeit in an infinite dimensional space. Attempted use of an ordinary gradient in place of a Sobolev gradient such a descent equation results in a partial differential equation which is likely to be more difficult to understand than (11.5). Contrast minimal surface development in Chapter 16 with codes that do evolution by mean curvature [24]. This comparison extends to a wide class of problems, problems such as that of Nash's embedding, [124]. Work on recasting Nash's work in terms of Sobolev gradients is in progress.

It will be seen in Chapter 12, that variational problems in $H^{m,p}$ for $1 < p < \infty$ but with $p \neq 2$, can be dealt with as in Section 11.3. Many of the considerations in the present chapter apply equally well to such non-Hilbert settings.

Chapter 12
An Introduction to Sobolev Gradients in Non-Inner Product Spaces

Many problems involving partial differential equations seem not to be placed naturally in Sobolev spaces $H^{m,p}(\Omega)$ for $p = 2$. Some important examples will be seen in Chapter 17 which deals with various transonic flow problems. In the present chapter Sobolev gradients in finite dimensional emulations of $H^{1,p}([0,1])$ are introduced for the case $p \neq 2$. Gradients are constructed with respect to a finite dimensional version of an $H^{m,p}$ space for $p > 1$. As such it provides us with an example of what might be regarded as another principle of gradient construction that could be added to the discussion in Chapter 1 and Chapter 9, the part concerning Riemannian metrics. See also the papers [183, 184] for closely related discussion of adjoint analysis.

Suppose H is a Hilbert space and ϕ is a C^1 function on H. Recall two equivalent ways to define a gradient of ϕ at x:

- $(\nabla\phi)(x)$ is the unique member y of H so that

$$(\phi'(x))h = \langle h, y\rangle_H,\ h \in H,\ \textit{and}$$

- $(\nabla\phi)(x)$ is the unique member y of H which maximizes

$$(\phi'(x))y \text{ is maximum subject to } \|y\|_H = |\phi'(x)|.$$

In Banach spaces which are not Hilbert spaces, the second alternative may be available whereas the first alternative is not. Specifically, suppose $\infty > p > 1$ and n denotes a positive integer. Then for a region Ω in R^m for some positive integer m, the second alternative is available where H is replaced by $H^{m,p}(\Omega)$ since this space is uniformly convex, ([86]). Our idea is illustrated in a finite dimensional version of $H^{1,p}([0,1])$:

For a positive integer n and $\delta = \frac{1}{n}$, denote by H the vector space whose points are those of R^{n+1} but with norm

$$\|y\|_H = (\sum_{i=0}^{n} |y_i|^p + \sum_{i=1}^{n} |\frac{1}{\delta}(y_i - y_{i-1})|^p)^{1/p},\ \ y = (y_0, y_1, ..., y_n) \in R^{n+1}. \tag{12.1}$$

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Define D_0, D_1, D as in (10.1), denote by $\alpha : R^n \times R^n \to R$ a C^2 function. Define $\phi : R^{n+1} \to R$ as follows,

$$\begin{aligned}\phi(y) &= \alpha(D_0 y, D_1 y)\\ &= \alpha(\frac{1}{2}(y_1+y_0), ..., \frac{1}{2}(y_n+y_{n-1})\frac{1}{\delta}(y_1-y_0), \ldots, \frac{1}{\delta}(y_n-y_{n-1})),\\ y &= (y_0, y_1, ..., y_n) \in R^{n+1}.\end{aligned}$$

Consider the problem of determining $h \in R^{n+1}$ so that

$$\phi'(y)h \text{ is maximum subject to } \|h\|_H^p - |\phi'(y)|^p = 0 \tag{12.2}$$

where

$$|\phi'(y)| = \sup_{g\in R^{n+1}, g\neq 0} |\phi'(y)g|/\|g\|_H.$$

Now some notation. Fix $y \in R^{n+1}$ and choose $A, B \in R^n$ so that the linear functionals

$$\alpha_1(D_0 y, D_1 y), \alpha_2(D_0 y, D_1 y)$$

have the representations

$$\begin{aligned}\alpha_1(D_0 y, D_1 y)k &= \langle k, A\rangle_{R^n}\\ \alpha_2(D_0 y, D_1 y)k &= \langle k, B\rangle_{R^n},\ k \in R^n.\end{aligned}$$

Then

$$\begin{aligned}\phi'(y)h &= \langle D_0 h, A\rangle_{R^n} + \langle D_1 h, B\rangle_{R^n}\\ &= \langle h, D_0^t A + D_1^t B\rangle_{R^{n+1}}\\ &= \langle h, q\rangle_{R^{n+1}},\ h \in R^{n+1}\end{aligned}$$

where

$$q = (\nabla\phi)(y) = D_0^t A + D_1^t B. \tag{12.3}$$

Proceed to find a unique solution to (12.2) and define a gradient of ϕ at $y, (\nabla_H \phi)(y)$, to be this solution. Note that there is some $h \in R^{n+1}$ which satisfies (12.2) since

$$\{h \in R^{n+1} : \|h\|_H^p = |\phi'(y)|^p\}$$

is compact. Define $\beta, \gamma : H \to R$ by

$$\beta(h) = \phi'(y)h,\ \gamma(h) = \|h\|_H^p - |\phi'(h)|^p,\ h \in R^{n+1}.$$

In order to use Lagrange multipliers to solve (12.2) first calculate conventional (*i.e.*, R^{n+1}) gradients of β, γ. Using (12.3),

$$(\nabla\beta)(h) = (D_0^t A + D_1^t B) = (\nabla\phi)(y) = q,\ h \in R^{n+1}.$$

Define Q so that $Q(t) = |t|^{p-2}, t \in R$. By direct calculation,

$$(\nabla\gamma)(h) = (\gamma^{(0)}(h), \gamma^{(1)}(h), \ldots, \gamma^{(n)}(h))$$

where

$$\begin{aligned}
\gamma^{(0)}(h) &= Q(h_0) - \frac{1}{\delta^2}Q(h_1 - h_0),\\
\gamma^{(n)}(h) &= Q(h_n) + \frac{1}{\delta^2}Q(h_n - h_{n-1}),\\
\gamma^{(i)}(h) &= Q(h_i) + \frac{1}{\delta^2}(Q(h_i - h_{i-1}) - Q(h_i - h_{i+1})),\\
&\quad i = 1, \ldots, n-1,\ h \in R^{n+1}.
\end{aligned}$$

This can be written more succinctly as

$$(\nabla\gamma)(h) = E^t(Q(Eh)) \tag{12.4}$$

where

$$E(h) = \left({}^{h}_{D_1 h}\right),\ h \in R^{n+1}$$

and the notation $Q(Eh)$ denotes the member of R^{n+1} which is obtained from Eh by taking Q of each of its components. The rhs of expression (12.4) gives a finite dimensional version of the p-Laplacian associated with the embedding of $H^{1,p}([0,1])$ into L_p and is denoted by $\Delta_p(h)$. Some references to p-Laplacians are [111].

The theory of Lagrange multipliers asserts that for any solution h to (12.2) (indeed of any critical point associated with that problem), it must be that $(\nabla\gamma)(h)$ and $(\nabla\beta)(h) = (\nabla\phi)(y)$ are linearly dependent. It will be seen that there are just two critical points for (12.2), one yielding a maximum and the other a minimum.

Lemma 12.1. *If $h \in R^{n+1}$ the Hessian of γ at $h, (\nabla\gamma)'(h)$, is positive definite unless $h = 0$. Moreover $(\nabla\gamma)'$ is continuous.*

Indication of proof. Using (12), for $h \in R^{n+1}$,

$$h \neq 0, (\nabla\gamma)'(h)$$

is symmetric and strictly diagonally dominant with positive entries on the diagonal. Thus $(\nabla\gamma)'(h)$ must be positive definite. Clearly $(\nabla\gamma)'$ is continuous.

Theorem 12.2. *If $g \in R^{n+1}$, there is a unique $h \in R^{n+1}$ so that*

$$(\nabla\gamma)(h) = g. \tag{12.5}$$

Moreover there is a number λ so that if $g = \lambda q$, then the solution h to (12.5) solves (12.2).

Proof. Since $(\nabla\gamma)'(h)$, $h \in R^{n+1}$, $h \neq 0$, is positive definite, it follows that γ is strictly convex. Now pick $g \in R^{n+1}$ and define

$$\eta(h) = \gamma(h) - \langle h, g\rangle_{R^{n+1}},\ h \in R^{n+1}. \tag{12.6}$$

Since γ is convex it follows that η is also convex. Noting that η is bounded below, it is seen that η has a unique minimum, say h. At this element h we have that

$$\eta'(h)k = \gamma'(h)k - \langle k, g\rangle_{R^{n+1}} = 0,\ k \in R^{n+1}. \tag{12.7}$$

Since $\gamma'(h)k = \langle(\nabla\gamma)(h), k\rangle_{R^{n+1}}$, it follows from (12.7) that

$$(\nabla\gamma)(h) = g. \tag{12.8}$$

□

At a critical point h of (12.2),

$$(\nabla\gamma)(h) = \lambda(\nabla\phi)(y)$$

for some $\lambda \in R$ and hence

$$\begin{aligned} h &= (\nabla\gamma)^{-1}(\lambda(\nabla\phi)(y)) \\ &= Q^{-1}(\lambda)(\nabla\gamma)^{-1}((\nabla\phi)(y)). \end{aligned}$$

The condition that $\beta(h) = 0$ determines λ up to sign; one choice indicating a maximum for (12.2) and the other a minimum (pick the one which makes $\phi'(x)h$ positive).

The above demonstrates a special case of the following (see [86]) as pointed out in [227]:

Theorem 12.3. *Suppose X is a uniformly convex Banach space, f is a continuous linear functional on X and $c > 0$. Then there is a unique $h \in X$ so that fh is maximum subject to $\|h\|_X = c$.*

The space H above (R^{n+1} with norm (12.1)) is uniformly convex. An argument for Theorem 12.2 gives rise to a constructive procedure for determining the solution of (12.8) in the special case (12.2). Higher dimensional analogues which generalize some of the material in Chapter 4 follow the lines of the present chapter with no difficulty. In [227] Zahran gives generalizations of a number of the propositions of Chapter 4 to spaces $H^{m,p}, p > 2$. In (12.4), the lhs does not depend on h and so that an effective solution of our maximization problem (12.2) depends on being able to solve, given $g \in R^{n+1}$, for h so that

$$\Delta_p(h) = g. \tag{12.9}$$

To this end there is a nonlinear version of the well-known Gauss-Seidel method (for solving symmetric positive definite linear systems) which may be used to solve (12.9), given $g = (g_0, \ldots, g_n) \in R^{n+1}$. Seek $h \in R^{n+1}$ so that

$$E^t(Q(E(h))) = g, \tag{12.10}$$

that is, so that

$$\begin{aligned}
\gamma^{(0)}(h) &= Q(h_0) - \frac{1}{\delta^2} Q(h_1 - h_0) = g_0, \\
\gamma^{(n)}(h) &= Q(h_n) + \frac{1}{\delta^2} Q(h_n - h_{n-1}) = g_n \\
\gamma^{(i)}(h) &= Q(h_i) + \frac{1}{\delta^2}(Q(h_i - h_{i-1}) - Q(h_i - h_{i+1})) = g_i, \\
&\quad i = 1, \ldots, n-1.
\end{aligned}$$

Now given $a, b, c \in R$, each of the equations individually

$$\begin{aligned}
Q(x) - \frac{1}{\delta} Q(a - x) &= b, \\
Q(x) + \frac{1}{\delta} Q(x - a) &= b, \\
Q(x) + \frac{1}{\delta^2}(Q(x - a) - Q(x - c)) &= b
\end{aligned}$$

has a unique solution x. Our idea for a nonlinear version of Gauss-Seidel for solving (12.10) consists in making an initial estimate for the vector h and then systematically updating each component in order by solving the relevant equation (using Newton's method), repeating until convergence is observed. Generalization to higher dimensional problems should be clear enough.

In [227] there are generalizations of some of the convergence results of Chapters 4,5 to uniformly convex spaces. In particular, there is a generalization of Theorem 4.5 in this direction. Some generalizations of parts of Theorem 5.4 are also in [227]. This reference contains an extensive discussion of the role of uniform convexity in defining Sobolev gradients on non-inner product spaces. Also included are some numerical experiments. See this publication for details.

Chapter 13
Singularities and a Simple Ginzburg-Landau Functional

Work in this section is joint with Robert Renka and is taken from [167]. Suppose $\epsilon > 0$ and d is a positive integer. Consider the problem of determining critical points of the functional ϕ_ϵ:

$$\phi_\epsilon(u) = \int_\Omega \frac{1}{2}(\|\nabla(u)\|^2 + \frac{1}{4\epsilon^2}(|u|^2-1)^2,\ u \in H^{1,2}(\Omega, C),\ u(z) = z^d,\ z \in \partial\Omega, \tag{13.1}$$

where Ω is the unit closed disk in C, the complex numbers. For each such $\epsilon > 0$, denote by $u_{\epsilon,d}$ a minimizer of (13.1).

In [20] it is indicated that for various sequences $\{\epsilon_n\}_{n=1}^\infty$ of positive numbers converging to 0, precisely d singularities develop for critical points $u_{\epsilon_n,d}$ as $n \to \infty$. The open problem is raised (Problem 12, page 139 of [20]) concerning possible orientation of such singularities. Our calculations suggest that for a given d there may be two resulting families of singularity configurations. Each configuration is formed by vertices of a regular $d-$gon centered at the origin of C, with each corresponding member of one configuration being about .6 times as large as a member of the other. A family of vortices is obtained by rotating a configuration through some angle α. That this results in another possible configuration follows from the fact (page 88 of [20]) that if

$$v_{\epsilon,d}(z) = e^{-id\alpha}u_{\epsilon,d}(e^{i\alpha}z), z \in \Omega,$$

then $\phi_\epsilon(v_{\epsilon,d}) = \phi_\epsilon(u_{\epsilon,d})$ and $v_{\epsilon,d}(z) = z^d, z \in \partial\Omega$.

That there should be vertex singularity patterns forming $d-$gons has certainly been anticipated although it seems that no proof has been put forward. What is offered here is some numerical support for this proposition. What is surprising in this work is the indication of *two* families for each positive integer d.

Here is an explanation of how these two families were encountered. Our calculations use steepest descent with numerical Sobolev gradients. One family appears using discrete steepest descent and the other appears when continuous steepest descent is closely tracked numerically. No explanation for this phenomenon if offered, but the results are simply reported. For a

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given d, the family of singularities obtained with discrete steepest descent is closer to the origin (by about a factor of .6) than the corresponding family for continuous steepest descent. In either case, the singularities found are closer to the boundary of Ω for larger d. A source of computational difficulties might be that critical points of ϕ_ϵ are highly singular objects (for small ϵ, a graph of $|u_{\epsilon,d}|^2$ would appear as a plate of height one above Ω with d slim tornadoes coming down to zero). Moreover for each d as indicated above, one expects a continuum of critical points (one obtained from another by rotation) from which to 'choose'.

For calculations the region Ω is broken into pieces using some number (180 to 400, depending on d) of evenly spaced radii together with 40 to 80 concentric circles.

For continuous steepest descent, using $d = 2, \ldots, 10$ a descent was started with a finite dimensional version of $u_{\epsilon,d}(z) = z^d,\ z \in C$. To emulate continuous steepest descent, a discrete steepest descent with small step size (on the order of .0001) was used in place of an optimal step size. In all runs reported on here $\epsilon = 1/40$ was used except for the discrete steepest descent run with $d = 2$. In that case $\epsilon = 1/100$ was used (for $\epsilon = 1/40$ convergence seemed not to be forthcoming in the single precision code used - the value .063 given is likely smaller than a successful run with $\epsilon = 1/40$ would give). Runs with somewhat larger ϵ yielded a similar pattern except the corresponding singularities were a little farther from the origin. In all cases there were found d singularities arranged on a regular d-gon centered at the origin.

Results for continuous steepest descent are indicated by the following pairs:

$$(2, .15), (3, .25), (4, .4), (5, .56), (6, .63), (7, .65), (8, .7), (9, .75), (10, .775)$$

where a pair (d, r) above indicates that a (near) singularity of $u_{\epsilon,d}$ was found at a distance r from the origin with $\epsilon = 1/40$. In each case the other $d - 1$ singularities are located by rotating the first one through an angle that is an integral multiple of $2\pi/d$.

Results for discrete steepest descent are indicated by the following pairs:

$$(2, .063), (3, .13), (4, .18), (5, .29), (6, .34), (7, .39), (8, .44), (9, .48), (10, .5)$$

using the same conventions as for continuous steepest descent. These numerical results are indicated in Figure 13.1. A plot of the square of the order parameter, for degree seven, is given in Figure 13.2.

Computations with a finer mesh would surely yield more precise results.

Some questions. Are there more than two (even infinitely many) families of singularities for each d? Does some other descent method (or some other method entirely) lead one to new configurations? Are there in fact configurations which are not symmetric about the origin?

Our thanks go to Pentru Mironescu for his description of this problem to the present writer in December 1996.

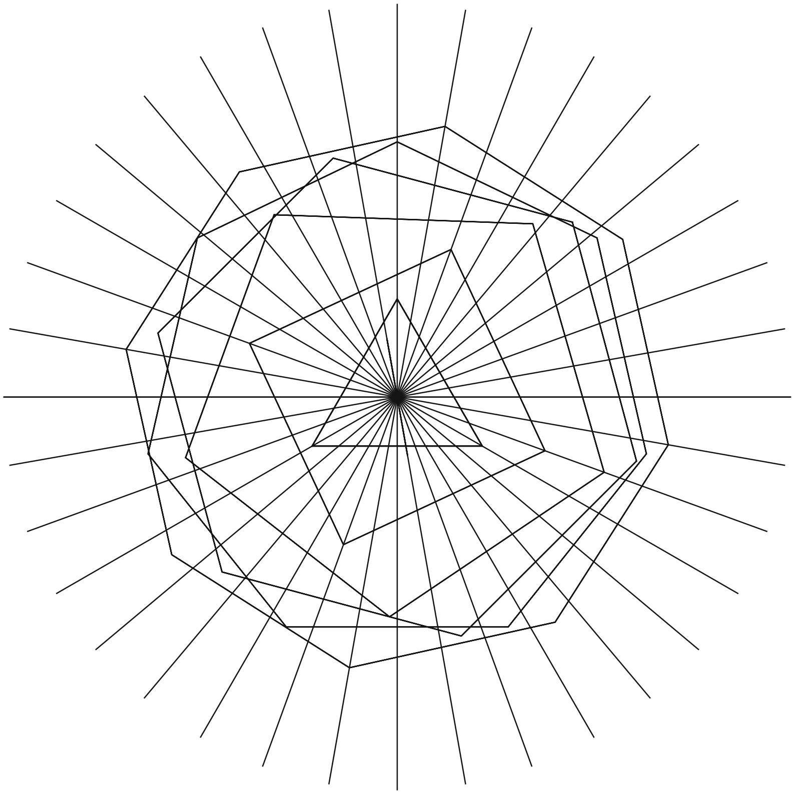


Fig. 13.1 Singularities for $d = 2, \ldots, 8$

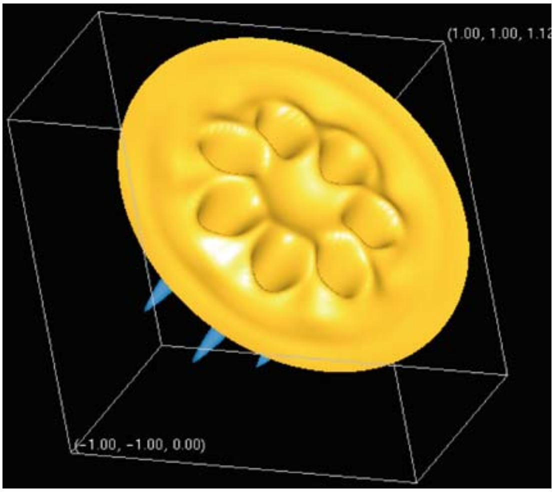


Fig. 13.2 Degree Seven Critical Point

Chapter 14
The Superconductivity Equations of Ginzburg-Landau

14.1 Introduction

Much of the work in this chapter contains joint work with Robert Renka, [139, 167, 191], and also recent work by P. Kazemi, [98]. There is considerable current interest in finding critical points of various forms of the Ginzburg-Landau (GL) functional. Such critical points give an indication of electron density and magnetic field associated with superconductors. We are indebted to Jacob Rubinstein for our introduction to this problem and have relied heavily on [54, 55, 209].

A method for determining such critical points numerically is presented and also some theoretical results are given.

14.2 A GL Functional and Its Sobolev Gradient

From [54, 55, 209], if $n = 2$ or 3, there is the following GL functional:

$$E(u, A) = \int_{\Omega} (\frac{1}{2}\|(\nabla - iA)u\|^2 + \frac{1}{2}\|\nabla \times A - H_0\|^2 + (\kappa^2 V(u)) \qquad (14.1)$$

where

$$V(z) = \frac{1}{4}(|z|^2 - 1)^2, z \in C.$$

The unknowns are

$$u \in H^{1,2}(\Omega, C), \quad A \in H^{1,2}(\Omega, R^n),$$

and the following are given to designate an imposed magnetic field and material constant, respectively:

$$H_0 \in C(\Omega, R^n), \quad \kappa \geq 0,$$

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_14,

and Ω denotes a bounded region in R^n with regular boundary. It is shown in [98] that (14.1) is well defined as a function from $H^{1,2}(\Omega, C) \times H^{1,2}(\Omega)$ into R.

In the following, take $n = 2$. To prepare for a discussion of numerics, change to real components. Take $D : H^{1,2}(\Omega)^4 \to L_2(\Omega, K)^{12}$ so that if $w = (r, s, a, b) \in H^{1,2}(\Omega)^4$, then

$$Dw = \begin{pmatrix} \binom{r}{\nabla r} \\ \binom{s}{\nabla s} \\ \binom{a}{\nabla a} \\ \binom{b}{\nabla b} \end{pmatrix}. \tag{14.2}$$

Denote by P the orthogonal projection of $L_2(\Omega)$ onto the range of D. To perhaps clarify this, denote by Q the orthogonal projection of $L_2(\Omega)^3$ onto

$$\{\begin{pmatrix} v \\ \nabla v \end{pmatrix} : v \in H^{1,2}(\Omega)\}.$$

Then for $\alpha, \beta, \gamma, \delta \in L_2(\Omega)^3$

$$P\begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} Q\alpha \\ Q\beta \\ Q\gamma \\ Q\delta \end{pmatrix}$$

Further following the above, define $F : R^{12} \to R$ so that if $w = (r, s, a, b) \in H^{1,2}(\Omega)$, then

$$F(Dw) = \frac{1}{2}(|r_1 + as|^2 + |s_1 - ar|^2 + |r_2 - bs|^2 + |s_2 - br|^2 \tag{14.3}$$

$$+ |b_2 - a_1 - H_0|^2) + \frac{\kappa^2}{4}(r^2 + s^2 - 1)^2, \tag{14.4}$$

(think $u = (r + is),\ A = \binom{a}{b}$.)

Rewrite (14.1) as

$$E(w) = \int_\Omega F(Dw),\ w \in H^{1,2}(\Omega)^4. \tag{14.5}$$

We seek to minimize (14.5) without imposing boundary conditions or other constraints on u, A in (14.5). To this end:

Lemma 14.1.

$$E'(w)h = \int_\Omega (F'(Dw))Dh,\ w, h \in H^{1,2}(\Omega)^4. \tag{14.6}$$

A careful examination of (14.6) reveals (see [98], Lemma 5.1), that $E'(w)$ is a continuous linear functional on $H^{1,2}$. In the above, F' denotes the Fréchet derivative of $F : R^{12} \to R$. Denoting by ∇F the gradient function for F, one can rewrite (14.6) as

$$E'(w)h = \int_{\Omega} \langle (\nabla F(Dw)), Dh \rangle_{R^{12}} \tag{14.7}$$

where the precise meaning of

$$(\nabla F)(w)$$

is that $(\nabla F)(w)$ has domain Ω and

$$((\nabla F)(w))(x) = (\nabla F)((Dw)(x)),\ x \in \Omega.$$

Since (14.7) gives that $E'(w)$ is a continuous linear transformation for each $w \in H^{1,2}(\Omega)^4$, there is ∇E from $H^{1,2}(\Omega)^4 \to$ into that space such that

$$E'(w)h = \langle h, (\nabla E)(w) \rangle_{H^{1,2}(\Omega)^4},\ w, h \in H^{1,2}(\Omega)^4.$$

The following gives a construction for ∇E.

Using Section 5.5, pick $p \in (1, 2)$ as indicated there for the choice of $n = 2$. Extend, as indicated in that section, P to $\hat{P}$ defined on $(L_p(\Omega) \times L_2(\Omega)^2)^4$.

Rewrite (14.7) as

$$E'(w)h = \langle Dh, ((\nabla F)(Dw)) \rangle_{L_2(\Omega)^{12}},\ w, h \in H^{1,2}(\Omega)^4.$$

Now $\hat{P}$ denotes the projection given in Theorem 5.5 (called simply P there) with the property that

$$\begin{aligned} \langle Dh, ((\nabla F)(Dw)) \rangle_{L_2(\Omega)^{12}} &= \langle \hat{P}(Dh), ((\nabla F)(Dw)) \rangle_{L_2(\Omega)^{12}} \\ &= \langle Dh, \hat{P}((\nabla F)(Dw)) \rangle_{L_2(\Omega)^{12}}. \end{aligned}$$

From this one sees that the first component of

$$(\nabla E)(w) = \hat{P}((\nabla F)(Dw)) \rangle_{L_2(\Omega)^{12}},$$

is the Sobolev gradient of E at w.

The above development contrasts with some previous treatments of the minimization problem for (14.5). In [54], for example, a Fréchet derivative for (14.1) is taken:

$$E'(u, A) \begin{pmatrix} v \\ B \end{pmatrix}, \quad u, v \in H^{1,2}(\Omega, C),\ A, B \in H^{1,2}(\Omega, R^2). \tag{14.8}$$

An integration by parts is performed resulting in the GL **equations** — the Euler-Lagrange equations associated with (14.1) together with the natural boundary conditions

$$(\nabla \times A) \times \nu = H_0 \times \nu, \quad ((\nabla - iA)u) \cdot \nu = 0 \tag{14.9}$$

on $\Gamma = \partial\Omega$ where ν is the outward unit normal function on Γ. Conventionally, one tries to solve the resulting Euler-Lagrange equations together with the above mentioned boundary conditions in order to arrive at a critical point. The GL equations here since they will not be needed here. See Chapter 11 for further discussion.

14.3 Finite Dimensional Emulation

Take Ω to be a square domain in R^2. Choose a positive integer n. Consider the rectangular grid Ω_n on Ω obtained by dividing each side of Ω into n pieces of equal length. Denote by H_n the collection of all functions from Ω_n to R^4. For $v \in H_n$, denote by $D_n v$ the proper analogue of (14.2) (values corresponding to divided differences are considered attached to centers of grid squares and function values at cell centers are obtained by averaging grid-point values). The calculations following (14.2) have their precise analogy in this finite dimensional setting: for F as used in (14.3), there is a function E_n which corresponds to a finite dimensional version of E in (14.3). Thus (14.3) corresponds to

$$E_n(w) = \sum_{i,j=1,\ldots,n} F((D_n w)_{(i,j)}, H_{0(i,j)}), \quad w \in H_n$$

which in turn gives that

$$\begin{aligned} E_n'(w)k &= \langle D_n k, (\nabla_1 F)(D_n w, H_0)\rangle_{J_n} \\ &= \langle k, D_n^t(\nabla_1 F)(D_n w, H_0)\rangle_{H_n'}, \quad w, k \in H_n. \end{aligned} \tag{14.10}$$

From (14.10) it follows that ∇E_n, the conventional gradient function for E_n, is specified by

$$(\nabla E_n)(w) = D_n^t(\nabla_1 F)(D_n w, H_0), \quad w \in H_n.$$

From (14.10) it follows that

$$E_n'(w)k = \langle k, \pi P_n(\nabla_1 F)(D_n w, H_0)\rangle_{H_n'}, \; w, k \in H_n.$$

Hence the Sobolev gradient function $\nabla_S E_n$ is given by

$$(\nabla_S E_n)(w) = \pi P_n (\nabla_1 F)(D_n w, H_0),\ w \in H_n.$$

To finish a description of how this Sobolev gradient is calculated note first that

$$P_n = D_n (D_n^t D_n)^{-1} D_n^t$$

since the range of P_n is a subset of the range of D_n, P_n is fixed on the range of D_n, P_n is symmetric and idempotent. This is enough to convict P_n of being the orthogonal projection onto the range of D_n. Thus

$$\begin{aligned}(\nabla_S E_n)(w) &= \pi D_n (D_n^t D_n)^{-1} D_n^t (\nabla_1 F)(D_n w, H_0) \\ &= (D_n^t D_n)^{-1} (\nabla E_n)(w)\end{aligned}$$

After computation of the standard gradient $\nabla E_n(w)$, an iterative (Gauss-Seidel) method (or other linear solver) is used to solve the symmetric positive definite linear system for the discretized Sobolev gradient.

14.4 Numerical Results

Here are some numerical results with which performance of Sobolev gradient can be compared to results using the ordinary gradient. As indicated in Chapter 2, one should expect much better results using the Sobolev gradient. The following table reflects this. Results are for two distinct runs, one using a Sobolev gradient and the second using a conventional gradient, for each of 5 values of n, the number of cells in each direction (Ω is partitioned into n^2 square cells). The following gives some timings for a typical set of runs:

	Sobolev gradient			Standard gradient		
n	SD steps	LS iterations	Time	SD steps	Time	Speedup
10	12	209	4	1049	36	9.0
20	16	542	16	3345	413	25.8
30	13	606	35	6579	1913	54.7
40	16	768	77	10591	5666	73.6
50	12	870	122	15275	12632	103.5

The columns labeled ‘SD steps’ contain the number of steepest descent steps, and the column labeled ‘LS iterations’ contains the total number of linear solver iterations. Since the condition number of the linear systems increases with n, so does the number of linear solver iterations per descent step. All times in are in seconds on an older PC. The column labeled ‘Speedup’ contains the ratios of execution times. Note that the relative advantage of the Sobolev gradient over the standard gradient increases with problem size.

Convergence is defined by an upper bound of 10^{-6} on the mean absolute (conventional) gradient component: $(n+1)^{-2}\|\nabla G_n(u,A)\|_{R^{(n+1)^2}}$. Parameter values are $\Omega = [0,1] \times [0,1], \kappa = 1., H_0(x,y) = 1., (x,y) \in \Omega$. The initial estimate in all cases was taken from $A = 0, u(x,y) = 1+i, (x,y) \in \Omega$. Linear systems were solved by a conjugate gradient method in which the convergence tolerance was heuristically chosen to decrease as the descent method approached convergence. The line search consisted of univariate minimization in the search direction (negative gradient direction). The number of evaluations of the functional per descent step averaged 26.2 with the Sobolev gradient and 8.4 with the conventional gradient.

The setting for Figure 14.1 is a sequence of holes in a superconductor. What is graphed there is the magnitude of the order parameter u. Here the top of the graph represents the pure superconducting state, $u = 1$. The bottom represents $u = 0$. The main feature is that a vortex is captured at the center of the row of holes. There is widespread interest in the superconductivity community concerning what combination of holes and moats (essentially pieces cut out of a superconductor) energetically attracts vortices. The idea is that if vortices (flux quanta) are attracted energetically to holes and motes, then some areas are left free of vortices - places in which superconducting circuits may be placed. When a slit or moat, rather than a collection of holes, is used, then one often sees flux quanta captured by the figure. These captures are represented by a circulation of superconducting electrons around the figure. It is of ongoing interest to make a simulator, using a code such

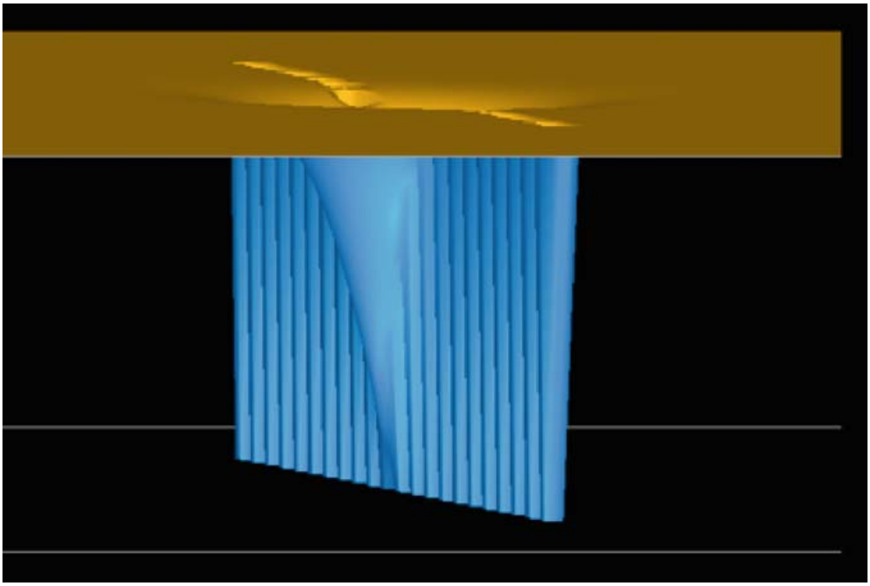
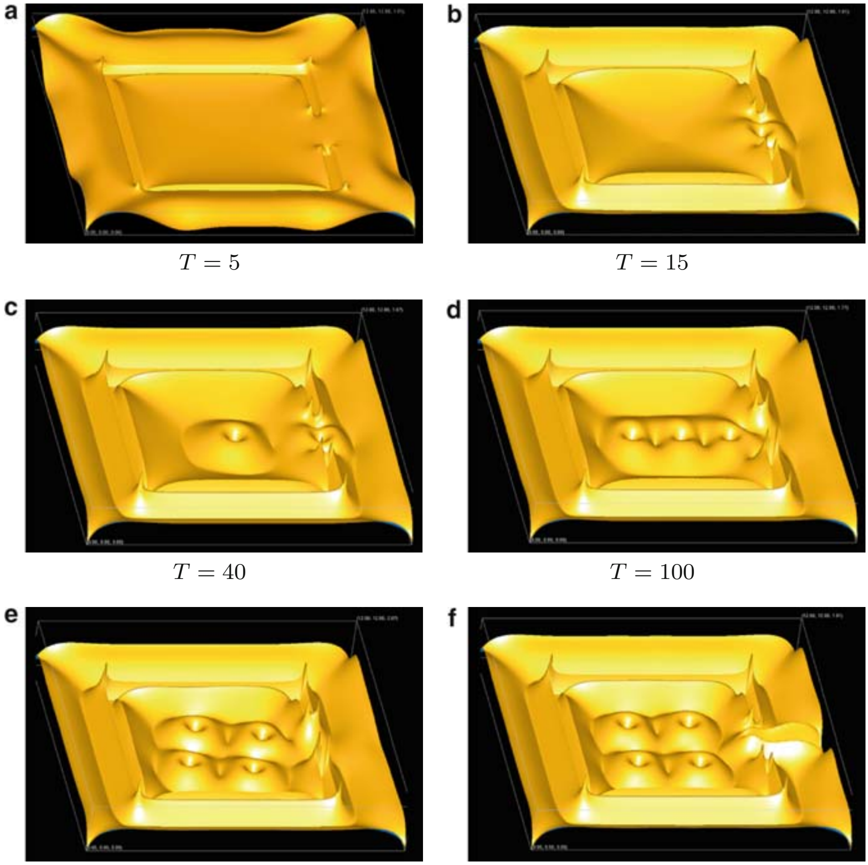


Fig. 14.1 Vortex Captured by a Line of Holes



a $T = 5$ b $T = 15$

c $T = 40$ d $T = 100$

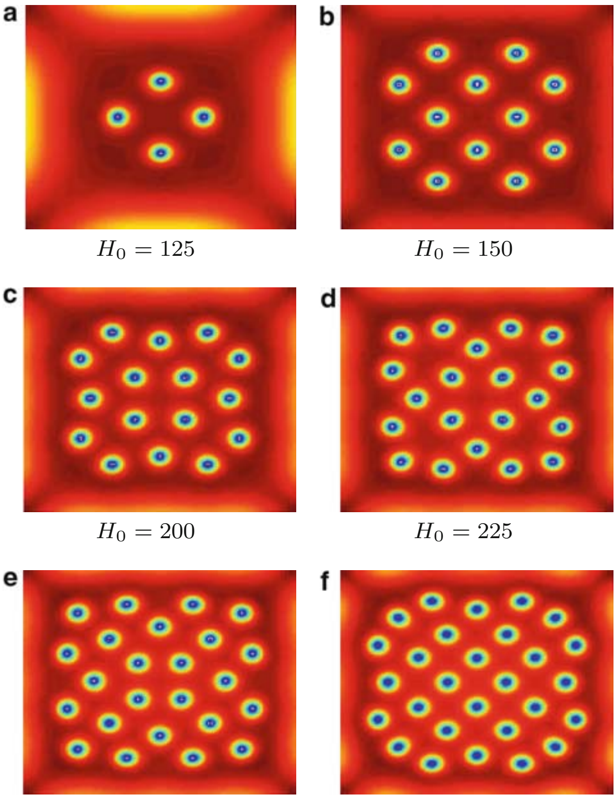
e $T = 200$ f $T = 1000$

Fig. 14.2 Magnitude of Magnetic Fields

as one that produced this figure. Such a simulator would allow an engineer to experiment computationally with many possible configurations in order to decide which ones are the most interesting to build.

In Figures 14.2, some plots by B. Neuberger are for a superconducting device which has a moat with a single bridge to the exterior part of the device. What is plotted is the magnitude of superconducting current. A time-dependent version of the GL equations is being solved, with reports at times $5, 15, 40, 100, 200, 1000$. In the progression in time, vortices are congregating inside of the moat. This suggests the possibility that such a moat might energetically attract vortices to the interior of the moat, possibly leaving the exterior of the moat free of vortices.

In Figure 14.3 there is a progression of contour plots of the order parameter for increasing magnetic fields. These plots were made by P. Kazemi and

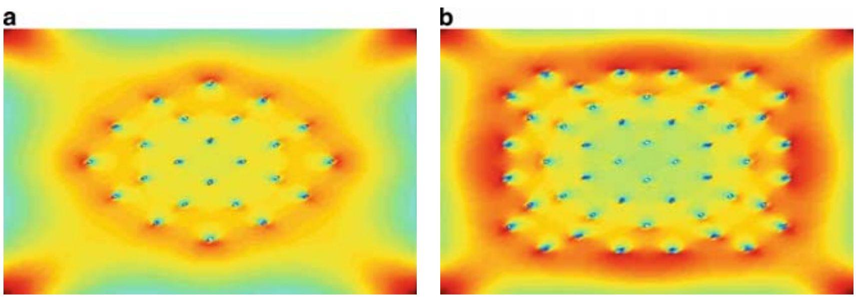


$H_0 = 125$ $H_0 = 150$

$H_0 = 200$ $H_0 = 225$

$H_0 = 250$ $H_0 = 275$

Fig. 14.3 Order Parameters Plots for $\kappa = 50$



$H_0 = 550$ $H_0 = 650$

Fig. 14.4 Order Parameters Plots for $\kappa = 200$

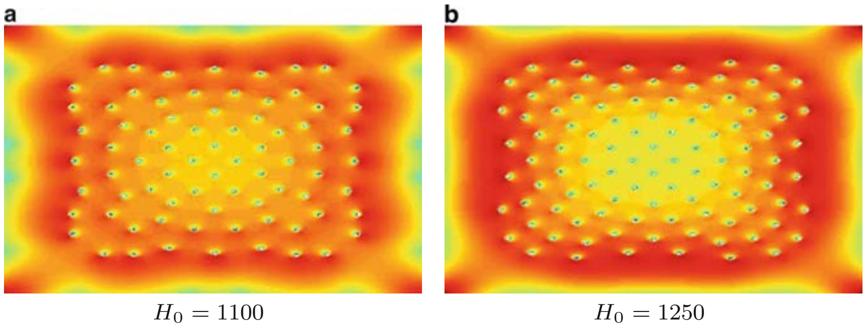


Fig. 14.5 Order Parameters Plots for $\kappa = 300$

appear in [98] for $\kappa = 50$. They demonstrate how, in the proper range, higher magnetic fields result in more tightly packed vortices. Figures 14.4, 14.5 are plots for still higher values of κ.

In [33] there is a finite element treatment of the GL equations of this chapter, including the time-dependent GL equations. A theoretical discussion and extensive numerical results, are given.

Chapter 15
Tricomi Equation: A Case Study

The Tricomi equation on a region Ω in R^2 is the problem of finding solutions u to

$$yu_{1,1}(x,y) + u_{2,2}(x,y) = 0,\ (x,y) \in \Omega. \tag{15.1}$$

This choice of $\Omega = [-1,1] \times [-1,1]$ yields a PDE which is elliptic in the upper half of Ω and hyperbolic in the lower half. On such a region, (15.1) serves as a prototype for 'mixed type' equations. It is considered to be a simple model for transonic flow, in which the part of Ω on which the solution is elliptic corresponds to subsonic flow and the hyperboic part corresponds to supersonic flow.

It is my understanding that despite considerable effort, there is not known a set of boundary conditions with respect to which (15.1) has one and only one solution. There are some special regions on which more is known, [114], but Tricomi's equation can never be said to be understood without dealing successfully with a region such as the present choice. See Chapters 8,19,20 for additional discussion of supplementary conditions. Additional aspects for the Tricomi and Burgers' equations are found in [99].

A Sobolev gradient steepest descent is used in order to gain insight into the set of solutions of (15.1). The function space for this problem is the Sobolev space $H = H^{2,2}(\Omega)$.

Define $\phi : H \to R$ by

$$\phi(u) = \frac{1}{2}\int_\Omega (\alpha u_{1,1} + \beta u_{2,2})^2,\ u \in H, \tag{15.2}$$

where

$$\alpha(x,y) = y, \beta(x,y) = 1,\ (x,y) \in \Omega.$$

Observe that the Fréchet derivative of ϕ is given by

$$\phi'(u)h = \int_\Omega (\alpha u_{1,1} + \beta u_{2,2})(\alpha h_{1,1} + \beta h_{2,2})\ u,h \in H. \tag{15.3}$$

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Resist the temptation to integrate by parts in (15.3). Given $u \in H$, seek $g \in H$ so that

$$\phi'(u)h = \langle h, g\rangle_H,\ h \in H. \tag{15.4}$$

Some more notation: For $u \in H$, $\overline{u}$ denotes the member

$$(u, u_1, u_2, u_{1,1}, u_{1,2}, u_{2,2}) \in L$$

where $L = (L_2(\Omega))^6$. Denote by $\pi : L \to H$ the transformation so that if $w \in L$, then πw is the first element of w. Denote by P the orthogonal projection of L onto its subspace

$$\{\overline{u} : u \in H\}.$$

Finally, if $u \in H$, Tu denotes

$$\alpha u_{1,1} + \beta u_{2,2}$$

and Fu denotes

$$(0, 0, 0, \alpha Tu, 0, \beta Tu).$$

Then (15.3) may be rewritten:

$$\phi'(u)h = \langle \overline{h}, Fu\rangle_L = \langle P\overline{h}, Fu\rangle_L = \langle \overline{h}, PFu\rangle_L,\ u, h \in H,$$

and hence

$$\phi'(u)h = \langle h, \pi PFu\rangle_H,\ u, h \in H.$$

Thus Sobolev gradient $\nabla\phi$ is the function from H to H so that

$$(\nabla\phi)(u) = \pi PFu.\ u \in H.$$

So for each $u \in H$, $(\nabla\phi)(u)$ represents $\phi'(u)$ in terms of the chosen inner product on H.

Theorem 15.1. *If $w \in H$, there is a unique function $z : [0, \infty) \to H$ so that*

$$z(0) = w,\ z'(t) = -(\nabla\phi)(z(t)),\ t \geq 0. \tag{15.5}$$

Moveover,

$$u = \lim_{t\to\infty} z(t) \tag{15.6}$$

exists and u is the nearest solution of (15.1) *to w in the metric of H.*

This follows from results in Chapter 3.

If one understood sufficiently the nature of the transformation which takes w in (15.5) to u in (15.6), then one would have some hold on the set of all solutions to (15.1). In such an event the question of boundary conditions for (15.1) might be less pressing. Pictures at the end of this chapter were obtained by a MatLab code corresponding to a discrete numerical version of (15.5).

15.1 Numerical Simulation for Tricomi's Equation

Take a discrete version ϕ_n of (15.2) using an $n+1 \times n+1$ grid for some positive integer n. For the resulting space of dimension $(n+1)^2$ use a finite dimensional version H_n of $H^{2,2}(\Omega)$. Calculate the ordinary gradient, calling it $\nabla_n \phi$. The sought after Sobolev gradient, $\nabla_{S,n}\phi_n$ then satifies

$$\phi_n'(u)h = \langle h, (\nabla_{S,n}\phi_n)(u)\rangle_{H_n},\ u, h \in H_n.$$

As in Chapter 5, an embedding operator is a finite dimensional version of

$$M : L_2\Omega \to H$$

which connects $\nabla\phi_n$ and $\nabla_{S,n}\phi_n$:

$$(\nabla_{S,n}\phi_n)(u) = M(\nabla\phi_n)(u),\ u \in H_n.$$

Once a Sobolev gradient $\nabla_{S,n}\phi$ is in place, steepest descent iteration is

$$u \to u - \delta(\nabla_{S,n}\phi)$$

where δ is chosen optimally at each step.

15.2 Experimenting With Boundary Conditions

To experiment with possible boundary conditions, one can modify M as indicated in Section 8.8 by weighting the Sobolev metric heavily at points at which one wants to preserve values of the initial estimate. This has the effect of giving a version of the Sobolev gradient that is nearly zero at elements corresponding to gird points at which one wants to preserve initial values throughout the iteration. If too many boundary conditions are specified, then ϕ_n can not be driven to zero. If too few boundary conditions are specified (or none at all for that matter), then different starts to the iiteration are very likely to produce different numerical solutions. A MatLab code tricomi2.m provides a means to investigate which boundary conditions (more accurately, supplemental conditions) might be adequate for specifying a unique solution. Tricomi2.m has the capability to essentially fix values at any desired gird

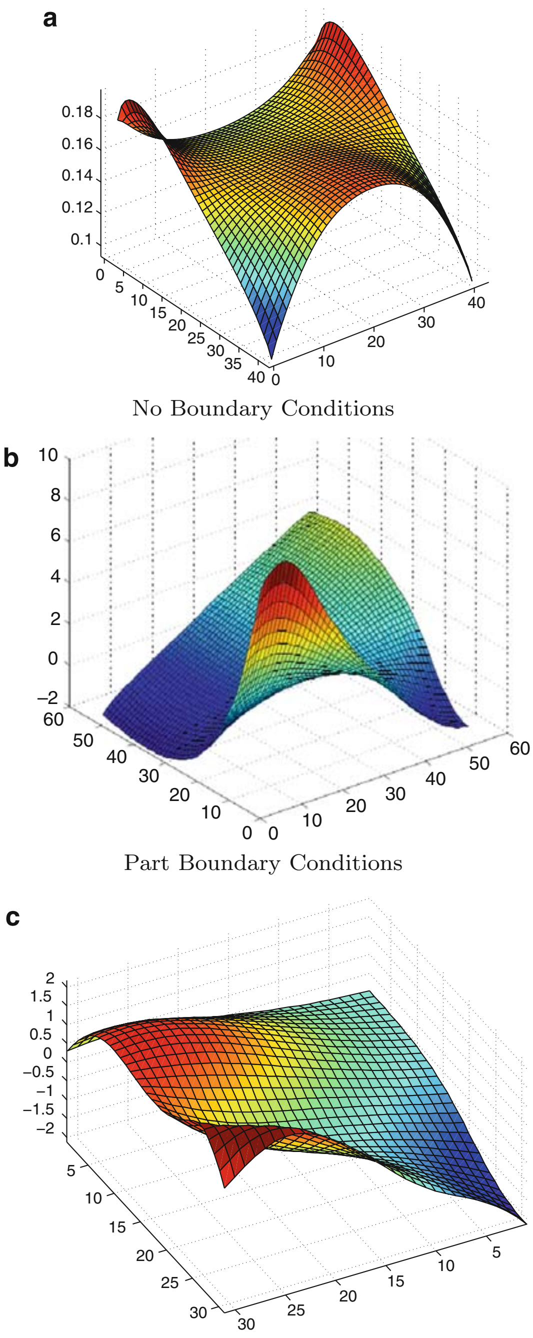

Fig. 15.1 Three Tricomi Plots

points. That such points need not be boundary grid points serves to broaden search possibilities. Various examples follow. A reader's is encouraged to obtain tricomi2.m or else write one themselves. A feature of this code is that in place of a numerical version of M above, M being the embedding operator between $L_2(\Omega)$ and $H^{2,2}(\Omega)$, the following was used: With $\hat{M}$ a numerical version of the embedding operator between $L_2(\Omega)$ and $H^{1,2}(\Omega)$, use $\hat{M}^2$ in place of the numerical version of M. This leads to simpler coding, but has an experimental aspect since the issue of corresponding natural boundary conditions for the resulting laplacian have not be entirely worked out (see section containing Theorem 5.5).

The three graphs in Figure 15.1 result from starting with various initial estimates. The first started with $u(x, y) = y(1 - y), (x, y) \in \Omega$, the second started with

$$u(x, y) = \frac{1}{.1 + (y - .1)^2}, (x, y) \in \Omega,$$

but the value of the initial estimate was required to be maintained on leading edge to the left. In the third graph, no boundary conditions were imposed but the start was $u(x, y) = \sin(x * y), (x, y) \in \Omega$. The orientation on the three graphs differ from each other, but with study a reader can distinguish the elliptic part from the hyperbolic part. In the hyperbolic part, curvatures in the X and Y directions are the same whereas in the elliptic part, curvatures in these two directions are of opposite signs.

See Kim [99] for some additional information on this problem.

Chapter 16
Minimal Surfaces

16.1 Introduction

This chapter discusses an approach to the minimal surface problem by means of a descent method using Sobolev gradients on a structure somewhat similar to a Hilbert manifold. It begins with a rather detailed discussion of the problem of minimal length between two fixed points. This problem, of course, has the obvious solution but it is hoped that the explicit calculation in this case will reveal some of our ideas. The work of this chapter is joint work with Robert Renka and is taken from [190].

16.2 Minimum Curve Length

Let S denote the set of smooth regular parametric curves on $[0, 1]$; i.e.,

$$S = \{f : f \in C^2([0, 1], \mathbf{R}^2) \text{ and } \|f'(t)\| > 0 \quad \forall\, t \in [0, 1]\},$$

where $\|\cdot\|$ denotes the Euclidean norm on $\mathbf{R}^2$. Denote curve length $\phi : S \to \mathbf{R}$ by

$$\phi(f) = \int_0^1 \|f'\| = \int_0^1 s',$$

where s is the arc length function associated with f; i.e.,

$$s(t) = \int_0^t \|f'\| \quad \forall\, t \in [0, 1].$$

Suppose that each of A and B is in R^2. It is sought to minimize ϕ over $f \in S$ so that $f(0) = A$ and $f(1) = B$. Pick $f \in S$ satisfying these end-point

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conditions. Variations are taken with functions that satisfy zero end conditions, that is consider perturbations h from:

$$S_0 = \{h : h \in C^2([0,1], \mathbf{R}^2) \text{ and } h(0) = h(1) = 0\}.$$

Then,

$$\begin{aligned}
\phi'(f)h &= \lim_{\alpha \to 0} \frac{1}{\alpha}[\phi(f + \alpha h) - \phi(f)] \\
&= \lim_{\alpha \to 0} \frac{1}{\alpha} \int_0^1 (\|f' + \alpha h'\| - \|f'\|) \\
&= \lim_{\alpha \to 0} \frac{1}{\alpha} \int_0^1 \frac{\|f' + \alpha h'\|^2 - \|f'\|^2}{\|f' + \alpha h'\| + \|f'\|} \\
&= \lim_{\alpha \to 0} \frac{1}{\alpha} \int_0^1 \frac{2\alpha\langle f', h'\rangle + \alpha^2\|h'\|^2}{\|f' + \alpha h'\| + \|f'\|} \\
&= \int_0^1 \langle f', h'\rangle / \|f'\| = \int_0^1 \langle f', h'\rangle / s', \\
&\qquad \forall\, h \in S_0. \qquad (16.1)
\end{aligned}$$

Note that $\phi'(f)h$ can be rewritten as a Stieltjes integral:

$$\phi'(f)h = \int_0^1 \langle f'/s', h'/s'\rangle\, s' = \int_0^1 \left\langle \frac{df}{ds}, \frac{dh}{ds} \right\rangle ds, \qquad (16.2)$$

where $\frac{df}{ds} = f'/s'$ and $\frac{dh}{ds} = h'/s'$ are the derivatives of f and h with respect to the arc length function s (associated with f). Thus $\phi'(f)h$ has been expressed in a parameter-independent way in the sense that both the Stieltjes (more accurately, the Hellinger) integral and the indicated derivatives depend only on the two curves involved and not on their parameterization.

A Hilbert space is obtained by defining an inner product on the linear space S_0. The gradient of ϕ at f depends on the chosen metric. First consider the standard L_2 norm associated with the inner product

$$\langle g, h\rangle_{(L_2[0,1])^2} = \int_0^1 \langle g, h\rangle \qquad \forall\, g, h \in S_0.$$

Integrating by parts (assuming for the moment that $f \in C^{(2)}$),

$$\begin{aligned}
\phi'(f)h &= \int_0^1 \langle f', h'\rangle / s' = \int_0^1 \langle f'/s', h'\rangle \\
&= \int_0^1 \langle -(f'/s')', h\rangle = \langle -(f'/s')', h\rangle_{(L_2[0,1])^2} \quad \forall\, h \in S_0.
\end{aligned}$$

Thus the representation of the linear functional $\phi'(f)$ in the L_2 metric is

$$\nabla\phi(f) = -(f'/s')'.$$

Note that the negative gradient direction (used by the steepest descent method) is toward the center of curvature; i.e.,

$$-\nabla\phi(f) = (f'/s')' = s'\kappa N$$

for curvature vector

$$\kappa N = \frac{d^2 f}{ds^2} = \frac{d}{ds}\left(\frac{f'}{s'}\right) = \frac{1}{s'}\left(\frac{f'}{s'}\right)' = \frac{f' \times f'' \times f'}{s'^4}.$$

Consider now a variable metric method in which the Sobolev gradient of ϕ at f is defined by an inner product that depends on f (but not the parameterization of f):

$$\langle k, h\rangle_f = \int_0^1 \langle k', h'\rangle / s' = \int_0^1 \left\langle \frac{dk}{ds}, \frac{dh}{ds}\right\rangle ds \quad \forall\, k, h \in S_0. \tag{16.3}$$

Let $k \in S_0$ denote the Sobolev gradient representing $\phi'(f)$ in this metric; i.e.,

$$\phi'(f)h = \langle k, h\rangle_f \quad \forall\, h \in S_0. \tag{16.4}$$

Then, from (16.1), (16.3), and (16.4),

$$\phi'(f)h = \int_0^1 \langle f', h'\rangle / s' = \int_0^1 \langle k', h'\rangle / s' \quad \forall\, h \in S_0$$

$$\Rightarrow \int_0^1 \left\langle \frac{f' - k'}{s'}, h' \right\rangle = -\int_0^1 \left\langle \left(\frac{f' - k'}{s'}\right)', h \right\rangle = 0 \quad \forall\, h \in S_0$$
$$\Rightarrow (f' - k')/s' = c \quad \text{for some } c \in \mathbf{R}^2.$$

Hence

$$k(t) = \int_0^t k' = \int_0^t (f' - cs') = f(t) - f(0) - cs(t),$$

where

$$k(1) = f(1) - f(0) - cs(1) = 0 \Rightarrow c = [f(1) - f(0)]/s(1)$$

i.e.,

$$f(t) - k(t) = f(0) + \frac{s(t)}{s(1)}[f(1) - f(0)] \quad \forall\, t \in [0, 1]. \tag{16.5}$$

The right hand side of (16.5) is the line segment between $f(0)$ and $f(1)$ parameterized by arc length s. Thus steepest descent with the Sobolev gradient k leads to the solution in a single iteration with step-size 1. While this remarkable result does not appear to extend to the minimal surface problem, our tests show that steepest descent becomes a viable method when the standard gradient is replaced by the (discretized) Sobolev gradient.

16.3 Minimal Surfaces

Denote the parameter space by $\Omega = [0,1] \times [0,1]$. The minimal surface problem is to find critical points of the surface area functional

$$\phi(f) = \int_\Omega \|f_1 \times f_2\|, \quad f \in C^1(\Omega, \mathbf{R}^3), \quad f_1 \times f_2 \neq 0,$$

(subject to Dirichlet boundary conditions) where f_1 and f_2 denote the first partial derivatives of f. This functional will be approximated by the area of a triangulated surface.

Define a triangulation T of Ω as a set of triangles such that

- No two triangles of T have intersecting interiors,
- The union of triangles of T coincides with Ω.
- No vertex of a triangle of T is interior to a side of a triangle of T.

Denote by V_T the set of all vertices of triangles of T, and let S_T be the set of all functions f from V_T to $\mathbf{R}^3$ such that, if $q - p$ and $r - p$ are linearly independent, then $f_q - f_p$ and $f_r - f_p$ are linearly independent for all $p, q, r \in V_T$ such that p is adjacent to q and r in the triangulation. Let Q be the set of all triples $\tau = [a, b, c] = [b, c, a] = [c, a, b]$ such that a, b,and c enumerate the vertices of a member of T in counterclockwise order. Denote the normal to a surface triangle by

$$f_\tau = (f_b - f_a) \times (f_c - f_a) = f_a \times f_b + f_b \times f_c + f_c \times f_a \quad \text{for } \tau = [a, b, c].$$

Note that $f_\tau \neq 0$ and the corresponding triangle area $\frac{1}{2}\|f_\tau\|$ is positive, where $\|\cdot\|$ now denotes the Euclidean norm on $\mathbf{R}^3$. Define surface area $\phi_T : S_T \to \mathbf{R}$ by

$$\phi_T(f) = \frac{1}{2} \sum_{\tau \in Q} \|f_\tau\|.$$

Now fix $f \in S_T$ and let $S_{0,T}$ denote the linear space of functions from V_T to $\mathbf{R}^3$ that are zero on the boundary nodes $V_T \cap \partial\Omega$. A straightforward calculation results in

$$\phi_T'(f)h = \frac{1}{2} \sum_{\tau \in Q} \langle f_\tau, (f, h)_\tau \rangle / \|f_\tau\| \quad \forall\, h \in S_{0,T}, \tag{16.6}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product on $\mathbf{R}^3$ and

$$\begin{aligned}(f, h)_\tau &= (f_b - f_a) \times (h_c - h_a) + (h_b - h_a) \times (f_c - f_a) \\ &= f_a \times h_b + h_a \times f_b + f_b \times h_c + h_b \times f_c \\ &\quad + f_c \times h_a + h_c \times f_a \quad \text{for } \tau = [a, b, c].\end{aligned}$$

It can be shown that the approximation to the negative L_2-gradient is proportional to the discretized mean curvature vector. Brakke has implemented a descent method based on this gradient [24]. However, for a metric on $S_{0,T}$, choose the one related to the following symmetric bilinear function which depends on f:

$$\langle g, h \rangle_f = \frac{1}{4} \sum_{\tau \in Q} \langle (f, g)_\tau, (f, h)_\tau \rangle \,/\, \|f_\tau\| \quad \forall\, g, h \in S_{0,T}. \tag{16.7}$$

It will be shown that, at least for a regular triangulation T of Ω, ((16.7) defines a positive definite function and hence an inner product). To this end, let n be a positive integer and consider the uniform rectangular grid with $(n+1)^2$ grid points $\{(i/n, j/n)\}_{i,j=0}^n$. Then let T_n denote the triangulation of Ω obtained by using the diagonal with slope -1 to partition each square grid cell into a pair of triangles.

Theorem 16.1. *For $f \in S_T$, $\quad T = T_n$, $\quad \langle \cdot, \cdot \rangle_f$ is positive definite on $S_{0,T}$.*

Proof. Suppose there exists $h \in S_{0,T}$ such that $\langle h, h \rangle_f = 0$. Then $(f, h)_\tau = 0\ \forall\, \tau \in Q$. It suffices to show that $h = 0$. Consider a pair of adjacent triangles indexed by $\tau_1 = [a, b, p]$ and $\tau_2 = [b, c, p]$ for which $h_a = h_b = h_c = 0$ so that

$$(f, h)_{\tau_1} = (f_b - f_a) \times h_p = 0 \text{ and } (f, h)_{\tau_2} = (f_c - f_b) \times h_p = 0.$$

For every such pair of triangles in T_n, a, b, and c are not collinear, and $f_b - f_a$ and $f_c - f_b$ are therefore linearly independent. Hence, being dependent on both vectors, $h_p = 0$. The set of vertices p for which $h_p = 0$ can thus be extended from boundary nodes into the interior of Ω. More formally, let $B_0 = V_T \cap \partial\Omega$ and denote by B_k the union of B_{k-1} with

$$\{p \in V_T : \exists\, a, b, c \in B_{k-1} \text{ such that } [a, b, p], [b, c, p] \in Q\}$$

for k as large as possible starting with $k = 1$. Then for some k, $B_k = V_T$ and, since $h_p = 0\ \forall\, p \in B_k$, it must be that $h = 0$. □

Let $g \in S_{0,T}$ denote the Sobolev gradient representing $\phi_T'(f)$ in the metric defined by (16.7); i.e.,

$$\phi_T'(f)h = \langle g, h \rangle_f \quad \forall\, h \in S_{0,T}. \tag{16.8}$$

Then from (16.6), (16.7), and (16.8),

$$\phi_T'(f)h = \frac{1}{2}\sum_{\tau\in Q}\langle f_\tau, (f,h)_\tau\rangle \,/\, \|f_\tau\| = \frac{1}{4}\sum_{\tau\in Q}\langle (f,g)_\tau, (f,h)_\tau\rangle \,/\, \|f_\tau\|$$

implying that

$$4\,\langle u,h\rangle_f = \sum_{\tau\in Q}\langle (f,u)_\tau, (f,h)_\tau\rangle \,/\, \|f_\tau\| = 0 \quad \forall\, h\in S_{0,T}, \tag{16.9}$$

where $u = f - g$ since

$$(f,u)_\tau = (f,f)_\tau - (f,g)_\tau = 2f_\tau - (f,g)_\tau.$$

For an alternative characterization of u, define $\beta(v) = \frac{1}{2}\|v\|_f^2\ \forall v\in S_T$, and let v be the minimizer of β over functions in S_T that agree with f on $\partial\Omega$. Then $\beta'(v)h = \langle v,h\rangle_f = 0\ \forall\, h\in S_{0,T}$. This condition is uniquely satisfied by $v = u = f - g$.

The Sobolev gradient g used in the descent iteration is obtained from u which is defined by (16.9). Expand the left hand side of (16.9) as follows. For $\tau = [a,b,c]$,

$$\begin{aligned}(f,u)_\tau &= u_a\times(f_b-f_c) + u_b\times(f_c-f_a) + u_c\times(f_a-f_b) \quad \text{and}\\ (f,h)_\tau &= h_a\times(f_b-f_c) + h_b\times(f_c-f_a) + h_c\times(f_a-f_b).\end{aligned}$$

Hence

$$\begin{aligned}\langle (f,u)_\tau,(f,h)_\tau\rangle &= \langle h_a,(f_b-f_c)\times(f,u)_\tau\rangle\\ &\quad + \langle h_b,(f_c-f_a)\times(f,u)_\tau\rangle + \langle h_c,(f_a-f_b)\times(f,u)_\tau\rangle\\ &= \langle h_a,(f_b-f_c)\times u_a\times(f_b-f_c) + (f_b-f_c)\\ &\quad \times[u_b\times(f_c-f_a) + u_c\times(f_a-f_b)]\rangle\\ &\quad + \langle h_b,(f_c-f_a)\times u_b\times(f_c-f_a) + (f_c-f_a)\\ &\quad \times[u_c\times(f_a-f_b) + u_a\times(f_b-f_c)]\rangle\\ &\quad + \langle h_c,(f_a-f_b)\times u_c\times(f_a-f_b) + (f_a-f_b)\\ &\quad \times[u_a\times(f_b-f_c) + u_b\times(f_c-f_a)]\rangle\end{aligned}$$

For $p\in V_T$, denote $\{\tau\in Q : p\in\tau\}$ by T^p. Then

$$\begin{aligned}&\sum_{\tau\in Q}\langle (f,u)_\tau,(f,h)_\tau\rangle \,/\, \|f_\tau\|\\ &= \sum_{p\in V_T}\langle h_p, \sum_{\tau=[p,b,c]\in T^p}\{(f_b-f_c)\times u_p\times(f_b-f_c)\\ &\quad + (f_b-f_c)\times[u_b\times(f_c-f_p) + u_c\times(f_p-f_b)]\}/\,\|f_\tau\|\rangle.\end{aligned}$$

From (16.9), this expression is zero for all $h \in S_{0,T}$. Thus

$$\sum_{\tau=[p,b,c]\in T^p} \{(f_b - f_c) \times u_p \times (f_b - f_c) + (f_b - f_c) \times [u_b \times (f_c - f_p) + u_c \times (f_p - f_b)]\} \|f_\tau\| = 0 \quad \forall p \in V_{I,T}, \tag{16.10}$$

where $V_{I,T}$ denotes the interior members of V_T. Equation (16.10) can also be obtained by setting $\frac{\partial \beta}{\partial u_p}$ to 0. In order to obtain an expression in matrix/vector notation, let $u = v + w$ where $v \in S_{0,T}$ and $w \in S_T$ is zero on $V_{I,T}$ (so that $v = u$ on $V_{I,T}$ and $w = u = f$ on the boundary nodes). Then (16.10) may be written

$$Au = q, \tag{16.11}$$

where

$$(A\mathbf{u})_p = \sum_{\tau=[p,b,c]\in T^p} \{(f_b - f_c) \times v_p \times (f_b - f_c) + (f_b - f_c) \times [v_b \times (f_c - f_p) + v_c \times (f_p - f_b)]\} / \|f_\tau\|$$

and

$$q_p = - \sum_{\tau=[p,b,c]\in T^p} (f_b - f_c) \times [w_b \times (f_c - f_p) + w_c \times (f_p - f_b)] \, / \, \|f_\tau\|$$

for all $p \in V_{I,T}$. For N interior nodes in $V_{I,T}$ and an arbitrarily selected ordering of the members of V_T, $\mathbf{u}$ and $\mathbf{q}$ denote the column vectors of length $3N$ with the components of u_p and q_p stored contiguously for each $p \in V_{I,T}$. Then A is a symmetric positive definite matrix with N^2 order-3 blocks. This follows from Theorem 16.1 since

$$\begin{aligned}
\mathbf{u}^T A\mathbf{u} &= \sum_{p\in V_{I,T}} \left\langle u_p, (A\mathbf{u})_p \right\rangle = \sum_{p\in V_T} \left\langle v_p, (A\mathbf{u})_p \right\rangle \\
&= \sum_{p\in V_T} \langle v_p, \sum_{\tau=[p,b,c]\in T^p} \{(f_b - f_c) \times v_p \times (f_b - f_c) \\
&\quad + (f_b - f_c) \times [v_b \times (f_c - f_p) + v_c \times (f_p - f_b)]\} / \|f_\tau\| \rangle \\
&= \sum_{\tau\in Q} \langle (f,v)_\tau, (f,v)_\tau \rangle \, / \, \|f_\tau\| = 4 \langle v, v \rangle_f \,.
\end{aligned}$$

Equation (16.11) may be solved by a block Gauss-Seidel or SOR method using $u = f$ as an initial solution estimate. No additional storage is required for the matrix (thus allowing for a large number of vertices), and convergence is guaranteed since A is positive definite [45, p. 72].

If f is sufficiently close to a local minimum of ϕ_T that second derivatives in all directions are positive, there is a Hessian inner product

$$\langle g,h\rangle_H = \phi_T''(f)gh = \frac{1}{2}\sum_{\tau\in Q}\frac{\langle (f,g)_\tau,(f,h)_\tau\rangle + \langle f_\tau,(g,h)_\tau\rangle}{\|f_\tau\|} - \frac{\langle f_\tau,(f,g)_\tau\rangle\langle f_\tau,(f,h)_\tau\rangle}{\|f_\tau\|^3},$$

for $g,\ h \in S_{0,T}$. The Hessian matrix H is defined by $\langle g,h\rangle_H = \langle Hg,h\rangle_{L_2}\ \forall g,h \in S_{0,T}$, and letting g now denote the H-gradient, g is related to the standard gradient $\nabla\phi_T(f)$ by $\phi_T'(f)h = \langle g,h\rangle_H = \langle Hg,h\rangle_{L_2} = \langle \nabla\phi_T(f),h\rangle_{L_2}\ \forall h \in S_{0,T}$, implying that $g = H^{-1}\nabla\phi_T(f)$. The displacement $u = f - g$ is obtained by minimizing

$$\langle u,u\rangle_H = \frac{1}{2}\sum_{\tau\in Q}\frac{\|(f,u)_\tau\|^2 + 2\langle f_\tau,u_\tau\rangle}{\|f_\tau\|} - \frac{\langle f_\tau,(f,u)_\tau\rangle^2}{\|f_\tau\|^3}$$

over functions u that agree with f on the boundary. Note that, for $g=0$, $\frac{1}{2}\langle u,u\rangle_f$ and $\frac{1}{2}\langle u,u\rangle_H$ are both equal to $\phi_T(f)$.

16.4 Uniformly Parameterized Surfaces

Numerical tests of the method revealed a problem associated with non uniqueness of the parameterization. Recall that, even in the minimum curve length computation, the parameterization of the solution depends on the initial curve. Thus, depending on the initial surface f_0, the method may result in a triangulated surface whose triangular facets vary widely in size and shape. Also, with a tight tolerance on convergence, the method often failed with a nearly null triangle (see Section 16.5). Currently available software packages such as EVOLVER [24] treat this problem by periodically retriangulating the surface (by swapping diagonals in quadrilaterals made up of pairs of adjacent triangles) during the descent process. As an alternative it was decided to add bounds on $\|f_\tau\|$ to the minimization problem. This finally led to a new characterization of the problem as described in the following two theorems.

Theorem 16.2. *Let*

$$\phi(f) = \int_\Omega \|f_1 \times f_2\|$$

and

$$\gamma(f) = \int_\Omega \|f_1 \times f_2\|^2$$

for $f \in C^2(\Omega, \mathbf{R}^3)$ *such that* $f_1 \times f_2 \neq 0$*. Then critical points of* γ *are critical points of* ϕ*; i.e., if*

$$\gamma'(f)h = 0 \,\forall\, h \in C_0^2(\Omega, \mathbf{R}^3) = \left\{h \in C^2(\Omega, \mathbf{R}^3\right) : h(x) = 0 \quad \forall\, x \in \partial\Omega\},$$

then

$$\phi'(f)h = 0 \,\forall\, h \in C_0^2(\Omega, \mathbf{R}^3).$$

Furthermore, such critical points f *are uniformly parameterized:* $\|f_1 \times f_2\|$ *is constant (and hence equal to the surface area* $\phi(f)$ *at every point since* Ω *has unit area).*

Proof. $\phi'(f)h = 0 \,\forall\, h \in C_0^2\left(\Omega, \mathbf{R}^3\right)$ if and only if

$$-\nabla\phi(f) = D_1\left(\frac{f_2 \times f_1 \times f_2}{\|f_1 \times f_2\|}\right) + D_2\left(\frac{f_1 \times f_2 \times f_1}{\|f_1 \times f_2\|}\right) = 0,$$

where D_1 and D_2 denote first partial derivative operators. (Note that the L_2-gradient $\nabla\phi(f)$ is proportional to the mean curvature of f.) Also,

$$\gamma'(f)h = 0 \,\forall\, h \in C_0^2\left(\Omega, \mathbf{R}^3\right)$$

if and only if

$$Lf = D_1\left(f_2 \times f_1 \times f_2\right) + D_2\left(f_1 \times f_2 \times f_1\right) = 0.$$

Thus it suffices to show that

$$Lf = 0 \Rightarrow \|f_1 \times f_2\|\, F$$

is constant. Expanding Lf,

$$\begin{aligned} Lf &= f_{12} \times (f_1 \times f_2) \,+\, f_2 \times D_1(f_1 \times f_2) \,+\, D_2(f_1 \times f_2) \,\times f_1 \\ &\quad + (f_1 \times f_2) \times f_{12} + f_2 \times D_1(f_1 \times f_2) \,+\, D_2(f_1 \times f_2) \times f_1 \\ &\quad + f_2 \times f_{11} \times f_2 \,+\, f_2 \times (f_1 \times f_{12}) \,+\, (f_{12} \times f_2) \times f_1 \\ &\quad + f_1 \times f_{22} \times f_1 \\ &= \langle f_2, f_2\rangle\, f_{11} - \langle f_2, f_{11}\rangle\, f_2 + \langle f_2, f_{12}\rangle\, f_1 - \langle f_1, f_2\rangle\, f_{12} \\ &\quad + \langle f_1, f_{12}\rangle\, f_2 - \langle f_1, f_2\rangle\, f_{12} + \langle f_1, f_1\rangle\, f_{22} - \langle f_1, f_{22}\rangle\, f_1, \end{aligned}$$

where the last equation follows from the identity

$$u \times (v \times w) = \langle u, w\rangle\, v - \langle u, v\rangle\, w.$$

Now suppose $Lf = 0$. Then $\langle f_1, Lf\rangle = \langle f_2, Lf\rangle = 0$ and hence

$$\begin{aligned}&\langle f_2 \times f_1 \times f_2, f_{11}\rangle + \langle f_1 \times f_2 \times f_1, f_{12}\rangle \\ &\quad = \langle f_2, f_2\rangle \langle f_1, f_{11}\rangle - \langle f_1, f_2\rangle \langle f_2, f_{11}\rangle \\ &\qquad + \langle f_1, f_1\rangle \langle f_2, f_{12}\rangle - \langle f_1, f_2\rangle \langle f_1, f_{12}\rangle = \langle f_1, Lf\rangle = 0\end{aligned}$$

and

$$\begin{aligned}&\langle f_2 \times f_1 \times f_2, f_{12}\rangle + \langle f_1 \times f_2 \times f_1, f_{22}\rangle \\ &\quad = \langle f_2, f_2\rangle \langle f_1, f_{12}\rangle - \langle f_1, f_2\rangle \langle f_2, f_{12}\rangle \\ &\qquad + \langle f_1, f_1\rangle \langle f_2, f_{22}\rangle - \langle f_1, f_2\rangle \langle f_1, f_{22}\rangle = \langle f_2, Lf\rangle = 0.\end{aligned}$$

Hence,

$$\begin{aligned}D_1\left(\|f_1 \times f_2\|\right) = {}& \frac{\langle f_1 \times f_2, D_1\left(f_1 \times f_2\right)\rangle}{\|f_1 \times f_2\|} \\ & - \frac{\langle f_2 \times f_1 \times f_2, f_{11}\rangle + \langle f_1 \times f_2 \times f_1, f_{12}\rangle}{\|f_1 \times f_2\|} = 0\end{aligned}$$

and

$$\begin{aligned}D_2\left(\|f_1 \times f_2\|\right) = {}& \frac{\langle f_1 \times f_2, D_2\left(f_1 \times f_2\right)\rangle}{\|f_1 \times f_2\|} \\ & - \frac{\langle f_2 \times f_1 \times f_2, f_{12}\rangle + \langle f_1 \times f_2 \times f_1, f_{22}\rangle}{\|f_1 \times f_2\|} = 0\end{aligned}$$

implying that $\|f_1 \times f_2\|$ is constant. □

The following theorem implies the converse of Theorem 16.2; i.e., critical points of ϕ are (with a change of parameters) critical points of γ. Note that the surface should not be confused with its representation by a parametric function.

Theorem 16.3. *Any regular parametric surface $f \in C^1(\Omega, \mathbf{R}^3)$ can be uniformly parameterized.*

Proof. Let $\alpha(x, y) = \|f_1(x, y) \times f_2(x, y)\|$, $(x, y) \in \Omega$, and define $\beta : \Omega \to \Omega$ by

$$\beta(x, y) = \begin{pmatrix} u(x, y) \\ v(x, y) \end{pmatrix}$$

where

$$u(x, y) = \frac{\int_0^x \alpha(r, y) dr}{\int_0^1 \alpha(r, y) dr}, \qquad v(x, y) = \frac{\int_0^y \int_0^1 \alpha(r, s) dr ds}{\phi(f)}.$$

Then

$$u_1(x,y) = \frac{\alpha(x,y)}{\int_0^1 \alpha(r,y)dr}, \quad v_1(x,y) = 0, \quad \text{and} \quad v_2(x,y) = \frac{\int_0^1 \alpha(r,y)dr}{\phi(f)}.$$

Note that $\phi(f) = \int_0^1 \int_0^1 \alpha(r,s)drds$, and by regularity of f, $\alpha(x,y) > 0$ $\forall\ (x,y) \in \Omega$. It is easily verified that β is invertible. Its Jacobian has determinant

$$u_1 v_2 - u_2 v_1 = \alpha/\phi(f).$$

Denote the reparameterized surface by

$$g(u,v) \equiv f\left(\beta^{-1}(u,v)\right).$$

Then $f(x,y) = g\left(\beta(x,y)\right)$ and

$$\begin{aligned} &f_1(x,y) \times f_2(x,y) \\ &\quad = \left[g_1(u,v)u_1(x,y) + g_2(u,v)v_1(x,y)\right] \times \left[g_1(u,v)u_2(x,y) + g_2(u,v)v_2(x,y)\right] \\ &\quad = (u_1 v_2 - u_2 v_1)\left[g_1(u,v) \times g_2(u,v)\right]. \end{aligned}$$

Hence $\|g_1(u,v) \times g_2(u,v)\| = \phi(f)$. □

Note that, in the analogous minimum curve length problem, the minimizer of $\int_0^1 \|f'\|^2$ satisfies $f'' = 0$ implying constant velocity resulting in a uniformly parameterized line segment, while the minimizer of $\int_0^1 \|f'\|$ satisfies $(f'/\|f'\|)' = 0$ implying zero curvature but not a uniform parameterization.

For the minimum curve length problem the analog of Theorem 16.2 holds in both the discrete and continuous cases, but this is not true of the minimal surface problem; i.e., the theorem does not apply to the triangulated surface. However, to the extent that a triangulated surface approximates a critical point of γ, its triangle areas are nearly constant. This is verified by our test results.

On the other hand, there are limitations associated with minimizing the discretization of γ. Forcing a uniformly triangulated surface eliminates the potential advantage in efficiency of an adaptive refinement method that adds triangles only where needed — where the curvature is large. Also, in generalizations of the problem, minimizing the discretization of γ can fail to approximate a minimal surface. In the case of three soap films meeting along a triple line, the triangle areas in each film would be nearly constant but the three areas could be different, causing the films to meet at angles other than 120 degrees. Furthermore, it is necessary in some cases of area minimization to allow surface triangles to degenerate and be removed.

It should be noted that, while similar in appearance, γ is not the Dirichlet integral of f, $\delta(f) = \frac{1}{2}\int_\Omega \|f_1\|^2 + \|f_2\|^2$, which is equal to $\phi(f)$ when f is a conformal map (f is parameterized so that $\|f_1\| = \|f_2\|$ and $\langle f_1, f_2\rangle = 0$) [49].

Minimizing δ has the advantage that the Euler equation is linear (Laplace's equation) but requires that the nonlinear side conditions be enforced by varying nodes of T.

The discretized functional to be minimized is

$$\gamma_T(f) = \frac{1}{4} \sum_{\tau \in Q} \|f_\tau\|^2, \quad f \in S_T,$$

and the appropriate inner product is

$$\langle g, h \rangle_f = \frac{1}{4} \sum_{\tau \in Q} \langle (f, g)_\tau, (f, h)_\tau \rangle \quad \forall\, g, h \in S_{0,T}.$$

Theorem 16.1 remains unaltered for this definition of $\langle \cdot, \cdot \rangle_f$. A Sobolev gradient g for γ_T is defined by $u = f - g$, where $\gamma_T'(f)h = \langle g, h \rangle_f$ implying that

$$\sum_{\tau \in Q} \langle (f, u)_\tau, (f, h)_\tau \rangle = 0 \quad \forall\, h \in S_{0,T},$$

and thus u satisfies (16.10) without the denominator $\|f_\tau\|$ (or with $\|f_\tau\|$ taken to be constant). The Hessian inner product associated with γ_T is

$$\langle g, h \rangle_H = \frac{1}{3} \gamma_T''(f) g h = \frac{1}{6} \sum_{\tau \in Q} \langle (f, g)_\tau, (f, h)_\tau \rangle + \langle f_\tau, (g, h)_\tau \rangle,$$

and the displacement is obtained by minimizing

$$\langle u, u \rangle_H = \frac{1}{6} \sum_{\tau \in Q} \|(f, u)_\tau\|^2 + 2 \langle f_\tau, u_\tau \rangle.$$

This expression is considerably simpler than the corresponding expression associated with ϕ_T.

16.5 Numerical Methods and Test Results

Fletcher Reeves nonlinear conjugate gradient method [64] was used with Sobolev gradients and step size obtained by a line search consisting of Brent's one dimensional minimization routine FMIN [67]. The number of conjugate gradient steps between restarts with a steepest descent iteration was taken to be 2. At each step, the linear system defining the gradient was solved by a block SOR method with relaxation factor optimal for Laplace's equation and the number of iterations limited to 500. Convergence of the SOR method was defined by a bound on the maximum relative change in a solution component between iterations. This bound was initialized to 10^{-3} and decreased by a factor of 10 (but bounded below by 10^{-13}) after each descent iteration in which the number of SOR iterations was less than 10, thus tightening the tolerance as the initial estimates improved with convergence of the descent method.

The SOR method was also used to solve the linear systems associated with attempted Newton steps. A Newton step was attempted if and only if the root-mean-square norm of the L_2 gradient at the previous iteration fell below a tolerance which was taken to be a decreasing function of n. Failure of the SOR method due to an indefinite Hessian matrix was defined as an increase in the Euclidean norm of the residual between any pair of consecutive iterations. In most cases this required only two wasted SOR iterations before abandoning the attempt and falling back to a conjugate gradient step. In some cases however, the number of wasted SOR iterations was as high as 20, and, more generally, there was considerable inefficiency caused by less than optimal tolerances.

The selection of parameters described above, such as the number of conjugate gradient iterations between restarts, the tolerance defining convergence of SOR, etc., were made on the basis of a small number of test cases and are not necessarily optimal. The Fletcher-Reeves method could be replaced by the Polak-Ribière method at the cost of one additional array of length $3(n+1)^2$. Also, alternative line search methods were not tried, nor was there any attempt to optimize the tolerance for the line search. However, again based on limited testing, conjugate gradient was not found to be substantially faster than steepest descent, and the total cost of the minimization did not appear to be sensitive to the accuracy of the line search. Adding a line search to the Newton iteration (a damped Newton method) was found to be ineffective, actually increasing the number of iterations required for convergence.

A regular triangulation $T = T_n$ of $\Omega = [0,1] \times [0,1]$ was used and the initial approximation f_0 was talem to be a displacement of a discretized minimal surface $f: \ f_0 = f + p$ for $f \in S_T, \ p \in S_{0,T}$. Note that f_0 defines the boundary curve as well as the initial value. The following three minimal surfaces $F \in C^\infty\left(\Omega, \mathbf{R}^3\right)$ were used to define f:

- **Catenoid** $F(x,y) = (R\cos\theta, R\sin\theta, y)$ for radius $R = \cosh(y - .5)$ and angle $\theta = 2\pi x$. The surface area is $\phi(F) = \int_\Omega \|F_1 \times F_2\| = \pi(1 + \sinh(1)) \cong 6.8336$.
- **Right Helicoid** $F(x,y) = (x\cos(10y), x\sin(10y), 2y)$ with surface area $\phi(F) = \sqrt{26} + \left[\ln\left(5 + \sqrt{26}\right)\right]/5 \cong 5.5615$.
- **Enneper's Surface** $F(x,y) = \left(\xi - \xi^3/3 + \xi\eta^2, \eta - \eta^3/3 + \xi^2\eta, \xi^2 - \eta^2\right)$ for $\xi = (2x-1)R/\sqrt{2}$ and $\eta = (2y-1)R/\sqrt{2}$, where $R = 1.1$. The surface area is $\phi(F) = 2R^2 + \frac{4}{3}R^4 + \frac{14}{45}R^6 \cong 4.9233$.

For each test function f, all three components were displaced by the discretization p of $P(x,y) = 100x(1-x)y(1-y)$ which is zero on $\partial\Omega$.

Table 16.1 Surface Areas and Iteration Counts, Low Accuracy

	$n = 10$	$n = 20$	$n = 30$	$n = 40$	$n = 50$
Catenoid $\phi_T(f)$	6.6986	6.7995	6.8184	6.8250	6.8281
$\phi(F) = 6.8336$					
Method 1					
Surface area	6.6984	6.8057	8.0053	8.0518	8.0593
CG (SOR) iterations	10(375)	20(996)	17(1538)	30(2648)	26(3766)
Newton iterations	0	0	0	0	0
RMS L_2 gradient	.15E-1	.74E-2	.33E0	.35E0	.28E0
Method 2					
Surface area	6.6964	6.8035	6.8219	6.8289	6.8352
CG (SOR) iterations	4(141)	11(435)	17(852)	15(1265)	21(1920)
Newton iterations	2(17)	0	0	0	0
RMS L_2 gradient	.36E-2	.86E-2	.45E-2	.48E-2	.45E-2
Helicoid $\phi_T(f)$	4.8409	5.3731	5.4771	5.5139	5.5310
$\phi(F) = 5.5615$					
Method 1					
Surface area	4.8139	5.3697	5.4801	5.5214	5.5397
CG (SOR) iterations	28(875)	20(971)	25(2670)	32(3856)	32(5170)
Newton iterations	0	0	0	0	0
RMS L_2 gradient	.36E-1	.76E-2	.15E-1	.12E-1	.15E-1
Method 2					
Surface area	4.8572	5.3820	5.4820	5.5170	5.5344
CG (SOR) iterations	4(137)	8(440)	15(1012)	20(1816)	41(6500)
Newton iterations	2(13)	2(25)	0	0	0
RMS L_2 gradient	.27E-1	.46E-2	.19E-2	.22E-2	.16E-1
Enneper $\phi_T(f)$	4.9077	4.9194	4.9215	4.9223	4.9227
Method 1					
$\phi(F) = 4.9233$					
Surface area	4.9118	4.9308	4.9311	4.9303	4.9581
CG (SOR) iterations	13(325)	12(846)	14(1493)	21(3134)	20(5753)
Newton iterations	0	0	0	0	0
RMS L_2 gradient	.11E-1	.17E-1	.88E-2	.15E-1	.34E0
Method 2					
Surface area	4.9139	4.9216	4.9228	4.9237	4.9245
CG (SOR) iterations	4(133)	15(674)	18(1231)	21(1743)	21(2470)
Newton iterations	2(24)	1(22)	0	0	0
RMS L_2 gradient	.63E-2	.16E-2	.14E-2	.13E-2	.11E-2

Table 16.1 displays the computed surface areas associated with minimizing $\phi_T(f)$ (method 1) and $\gamma_T(f)$ (method 2), for each test function and each of five values of n. Convergence of the descent method was defined by a bound of $.5 \times 10^{-4}$ on the relative change in the functional between iterations. The number of conjugate gradient iterations and the total number of SOR iterations (in parentheses) for each test case is displayed in the row labeled CG (SOR) iterations. Similarly, the number of Newton iterations is followed

by the total number of SOR iterations (for all Newton steps) in parentheses. Note that the cost of each SOR iteration is proportional to n^2 (with a smaller constant for method 2). Although each SOR step has a higher operation count (by a factor of 2 with method 1 and 1.5 with method 2) for a Newton iteration than a conjugate gradient iteration, this is offset by the fact that no line search is required for the Newton iteration. Method 2 is more efficient in all cases except the helicoid with $n = 50$. This is further discussed below. The rows labeled RMS L_2 gradient display the root-mean-square Euclidean norms of the L_2 gradients of the surface area ϕ_T.

The table also displays the triangulated surface areas $\phi_T(f)$ associated with the undisplaced surfaces. From these values, the discretization error is verified to be of order $\left(\frac{1}{n}\right)^2$; i.e., $n^2 \left|\phi(F) - \phi_T(f)\right|$ approaches a constant with increasing n, where $T = T_n$ and f is the discretization of F. Note, however, that the computed surface areas do not closely match the ϕ_T values and are in some cases smaller because, while both are triangulated surface areas with the same boundary values, the former are minima of the discretized functionals while the latter have nodal function values taken from smooth minimal surfaces.

The tabulated surface areas reveal some anomalies associated with non uniqueness of the solution. In the case of the catenoid, there is a second surface satisfying the same boundary conditions: a pair of parallel disks connected by a curve. This surface has an approximate area of 7.9893. Plots verify that it is this surface that is approximated by method 1 with $n = 30$, 40, and 50. The curve connecting the disks is approximated by long thin triangles. Assume that the nearly constant triangle area maintained by method 2 prevented it from converging to this solution. Additional tests on Enneper's surface with a larger domain (ξ and η in the range -2 to 2) revealed the apparent existence of a second minimal surface with the same boundary but with smaller surface area. Non-uniqueness of Enneper's surface was noted by Nitsche ([171]) .

Table 16.2 displays the same quantities as in Table 16.1 but with convergence tolerance 1.0×10^{-14}. The computed solutions are not significantly more accurate, but the tests serve to demonstrate the deficiencies of method 1 and the robustness of method 2. Method 1 failed to converge in all cases except the catenoid with $n = 10$ and $n = 20$ and Enneper's surface with $n = 10$. In all other cases the procedure was terminated when the minimum triangle area fell below 100ϵ for machine precision ϵ ($.222 \times 10^{-15}$). (Allowing the procedure to continue would have resulted in failure with a nearly singular linear system or a triangle area of 0.) Method 2, on the other hand, failed to converge only on the helicoid with $n = 50$. Table 2 displays the result of 500 iterations, but another 500 iterations resulted in no improvement. Pictures reveal a uniformly triangulated surface but with long thin triangles apparently caused by the tendency of triangle sides to be aligned with the lines of curvature. Also, for method 2, the ratio of largest to smallest triangle area is

Table 16.2 Surface Areas and Iteration Counts, High Accuracy

	$n = 10$	$n = 20$	$n = 30$	$n = 40$	$n = 50$
Catenoid $\phi_T(f)$	6.6986	6.7995	6.8184	6.8250	6.8281
$\phi(F) = 6.8336$					
Method 1					
Surface area	6.6962	6.7993	7.9922	8.0468	8.0435
CG (SOR) iterations	15(441)	498(13532)	104(5467)	82(4746)	95(8992)
Newton iterations	8(118)	8(790)	0	0	0
RMS L_2 gradient	.25E-7	.49E-8	.29E0	.35E0	.27E0
Method 2					
Surface area	6.6964	6.7994	6.8184	6.8251	6.8320
CG (SOR) iterations	4(141)	17(582)	69(2976)	122(5702)	180(7877)
Newton iterations	7(45)	10(138)	8(294)	6(540)	2(1000)
RMS L_2 gradient	.36E-2	.65E-3	.21E-3	.92E-4	.21E-2
Helicoid $\phi_T(f)$	4.8409	5.3731	5.4771	5.5139	5.5310
$\phi(F) = 5.5615$					
Method 1					
Surface area	4.8043	5.3632	5.4731	5.5127	5.5314
CG (SOR) iterations	192(13915)	384(10462)	785(23897)	572(30088)	311(15319)
Newton iterations	0	0	0	0	0
RMS L_2 gradient	.27E0	.26E-1	.29E-1	.66E-1	.87E-2
Method 2					
Surface area	4.8571	5.3821	5.4817	5.5163	5.5333
CG (SOR) iterations	4(137)	8(440)	104(4486)	209(10817)	500(62376)
Newton iterations	7(51)	11(119)	6(356)	5(1035)	0
RMS L_2 gradient	.27E-1	.46E-2	.14E-2	.83E-3	.16E-1
Enneper $\phi_T(f)$	4.9077	4.9194	4.9215	4.9223	4.9227
$\phi(F) = 4.9233$					
Method 1					
Surface area	4.9077	4.9197	4.9244	4.9242	4.9417
CG (SOR) iterations	172(4699)	933(41510)	146(4672)	372(20615)	37(6841)
Newton iterations	13(879)	0	0	0	0
RMS L_2 gradient	.29E-7	.16E-2	.79E-2	.71E-2	.34E0
Method 2					
Surface area	4.9138	4.9216	4.9227	4.9230	4.9231
CG (SOR) iterations	4(133)	15(674)	41(3527)	107(9024)	371(38551)
Newton iterations	12(128)	13(483)	20(3025)	11(3997)	11(4118)
RMS L_2 gradient	.63E-2	.14E-2	.65E-3	.36E-3	.22E-3

at most 5 in all cases other than the helicoid with $n = 50$, in which the ratio is 46 with the larger convergence tolerance and 98 with the smaller tolerance. In no case was a saddle point encountered with either method.

Excluding the cases in which the method failed to converge, the number of descent steps and the number of SOR steps per descent step both increase with n for all test functions and both the conjugate gradient and Newton methods, implying that the Hessian matrices and their approximations become increasingly ill-conditioned with increasing n. This reflects the fact that finite element approximations to second-order elliptic boundary value problems on two-dimensional domains result in condition numbers of O(N) for N nodes.

The small iteration counts demonstrate the effectiveness of the preconditioner for both methods. Additional tests revealed that the standard steepest descent method (using the discretized L_2 gradient) fails to converge unless the initial estimate is close to the solution. Also, the conjugate gradient method without preconditioning is less efficient than preconditioned steepest descent even when starting with a good initial estimate.

16.6 Conclusion

We have described an efficient method for approximating parametric minimal surfaces. In addition to providing a practical tool for exploring minimal surfaces, the method serves to illustrate the much more generally applicable technique of solving PDE's via a descent method that employs Sobolev gradients, and it demonstrates the effectiveness of such methods. Furthermore, it serves as an example of a variable metric method.

The implementations of method 1 (`MINSURF1`) and method 2 (`MINSURF2`) are available as Fortran software packages which can be obtained from netlib.

Chapter 17
Flow Problems and Non-Inner Product Sobolev Spaces

17.1 Full Potential Equation

From [88] we have the following one-dimensional flow problem. Consider a horizontal nozzle of length two which has circular cross sections perpendicular to its main axis and is a figure of revolution about its main axis. We suppose that the cross sectional area is given by

$$A(x) = .4[1 + (1 - x^2)],\ 0 \le x \le 2.$$

We suppose also that pressure and velocity depend only on the distance along the main axis of the nozzle and that for a given velocity u the pressure is given by

$$p(u) = [1 + ((\gamma - 1)/2)(1 - u^2)]^{\gamma/(\gamma-1)}$$

for all velocities for which $1 + ((\gamma - 1)/2)(1 - u^2) \ge 0$. Choose $\gamma = 1.4$, the specific heat corresponding to air. Define a density function m by

$$m(u) = -p'(u), u \in R.$$

Further define

$$J(f) = \int_0^2 Ap(f'),\ f \in H^{1,7}. \tag{17.1}$$

For general $\gamma > 1$ choose $H^{1,2\gamma/(\gamma-1)}$ in order that the integrand of (17.1) be in $L_1([0, 2])$. Thus the specific heat of the media considered determines the appropriate Sobolev space; for $\gamma = 1.4$, $2\gamma/(\gamma - 1) = 7$.

Taking a first variation,

$$J'(f)h = -\int_0^2 Am(f')h',\ f, h \in H^{1,7} \tag{17.2}$$

where the perturbation $h \in H^{1,7}$ is required to satisfy $h(0) = 0 = h(2)$ and f is required to satisfy

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_17,

$$f(0) = 0, f(2) = c \tag{17.3}$$

for some fixed positive number c. Denote

$$H_0 = H_0^{1,7}([0,2]) = \{h \in H^{1,7}([0,2]) : h(0) = 0 = h(2)\}.$$

Suppose $f \in H^{1,7}([0,2])$. By Theorem 12.3 there is a unique $h \in H_0$ such that

$$J'(f)h$$

is maximum subject to

$$\|h\| = |J'(f)|$$

where $|J'(f)|$ is the norm of $J'(f)$ considered as a member of the dual of H^*. This maximum $h \in H$ is denoted by $(\nabla_H J)(f)$, the Sobolev gradient of J at f. Later in this chapter there is constructed a finite dimensional emulation of this gradient. First it is pointed out some peculiar difficulties that a number of flow problems share with this example.

From (17.2), if $Am(f')$ were to be differentiable, one would arrive at an Euler equation:

$$(Am(f'))' = 0 \tag{17.4}$$

for f a critical point of J. Furthermore, given sufficient differentiability, one would have

$$A'm(f') + Am'(f')f'' = 0$$

for f a critical point of J. Observe that for some f, the equation (17.4) may be singular if for some

$$x \in [0,2],\ m'(f'(x)) = 0.$$

This simple appearing example leads to a differential equation (17.4) which has the particularly interesting feature that it might be singular depending on the whims of the nonlinear coefficient of f''. Some calculation reveals that this is exactly the case at $x \in [0,2]$ if $f'(x) = 1$ which just happens to be the case at the speed of sound for this problem ($f'(x)$ is interpreted as the velocity corresponding to f at x). It turns out that the choice of c in (17.3) determines the nature of critical points of (17.1) - in particular whether there will be transonic solutions, i.e., solutions which are subsonic for x small enough ($f'(x) < 1$) and then become supersonic ($f'(x) > 1$) for some larger x.

It is common that there are many critical points of (17.1). Suppose we have one, denoted by f. An examination of m yields that for each choice of a value of $y \in [0,1]$, there are precisely two values

$$x_1, x_2 \in [0, ((\gamma+1)/(\gamma-1))^{1/2}) \text{ so that } x_1 < x_2$$

and $m(x_1) = y = m(x_2)$. The value x_1 corresponds to a subsonic velocity and x_2 corresponds to a supersonic velocity. So if f is such that

$$0 < f'(t_1) < 1,\ 0 < f'(t_2) > 1 \text{ for some } t_1, t_2 \in [0,2],$$

and (17.3) holds, then additional solutions may be constructed as follows:

Pick two subintervals $[a,b], [c,d]$ of $[0,2]$ so that f is subsonic on [a,b] and supersonic on [c,d]. Define g so that it agrees with f on the complement of the union of these two intervals so that g' on $[a,b]$ is the supersonic value which corresponds as in the preceding paragraph to the subsonic values of f' on $[a,b]$. Similarly, take g' on $[c,d]$ to have the subsonic values of f' on $[c,d]$. Do this in such a way that

$$\int_0^2 f' = \int_0^2 g'.$$

In this way one may construct a large family of critical points g from a particular one f. Now at most one member of this family is a physically correct solution if one imposes the conditions that the derivative of a such a solution does not shock 'up' in the sense that going from left to right (the presumed flow direction) there is no point of discontinuity of the derivative that jumps from subsonic to supersonic. A discontinuity in a derivative which goes from supersonic to subsonic as one moves from left to right is permitted.

How a descent scheme can pick out a physically correct solution given the possibility of an uncountable collections of non-physical solutions.

A reply is the following: Take the left hand side of (17.4) and add an artificial dispersion, that is pick $\epsilon > 0$ and consider the problem of finding f so that

$$-(Am(f'))' + \epsilon f''' = 0. \tag{17.5}$$

Turn now to a numerical emulation of this development. Equation (17.5) is no longer singular. A numerical scheme for (17.5) may be constructed using the ideas of Chapter 10. Denote by w a numerical solution to (17.5) (on a uniform grid on $[0,2]$ with n pieces) satisfying the indicated boundary conditions. Denote by J_n the numerical functional corresponding to J on this grid. Denote by H_n the space of real-valued functions on this grid where the expression (12.1) is taken for a norm on H_n. Using the development in Chapter 12, denote the $H^{1,7}([0,2])$ Sobolev gradient of J_n at $v \in H_n$ by $(\nabla J_n)(v)$. Consider the steepest descent process

$$w_{k+1} = w_k - \delta_k (\nabla J_k)(w_k),\ k = 1, 2, \ldots \tag{17.6}$$

where $w_1 = w$, our numerical solution indicated above and for $k = 1, 2, \ldots, \delta_k$ is chosen optimally. We do not have a convergence proof for this iteration but do call attention to Figure 17.2 at the end of this chapter which shows two graphs superimposed. The smooth curve is a plot of w satisfying (17.5). The graph with the sharp break is the limit of $\{w_k\}_{k=1}^{\infty}$ of the sequence (17.6). The process picks out the one physically viable critical point (17.1). The success of this procedure seems to rest on the fact that the initial value w, the viscous solution, has the correct general shape. The iteration (17.6) then picks out a nearest, in some sense, solution to w which is an actual critical point of (17.1). A reader will recognize the speculative nature of the above 'assertions'; this writer would be quite pleased to be able to offer a complete formulation of this problem together with complete proofs, but we must be content here to raise the technical and mathematical issues concerning this approach to the problem of transonic flow. Results as indicated in Figure 17.2 are in good agreement with those of F. T. Johnson [88] of Boeing, to whom great appreciation is expressed for his posing this problem and for his considerable help and encouragement.

A similar development has been coded for a two dimensional version:

$$J(u) = \int_{\Omega} (1 + ((\gamma - 1)/2)|\nabla u|^2)^{\gamma/(\gamma-1)} \tag{17.7}$$

$u \in H^{1,7}(\Omega)$, where Ω is a square region in R^2 with a NACA-12 airfoil removed. Details follow closely those for the nozzle problem outlined above. Results are presented for two runs, one where air speed 'at infinity' is subsonic. Two plots are in Figure 17.2. In the first, airspeed at infinity is Mach .8, which is subsonic. In the second plot, airspeed at infinity is Mach 1.1, which is supersonic. In the first run one sees supersonic pockets built up on the top and bottom of the airfoil; in the second run one sees a subsonic stagnation region on the leading edge of the airfoil. Both are expected by those familiar with transonic flow problems.

Calculations in the two problems were straight 'off the shelf' in that procedures outlined in Chapter 12 were followed closely (with appropriate approximations being made on the airfoil to simulate zero Neumann boundary conditions there). It is this writer's belief that the same procedure can be followed in three dimensions. Our point is that procedures of this chapter are straightforward and that there should be no essential difficulties in implementing them in large scale three dimensional problems in which 'shock fitting' procedures would be daunting (we claim the procedure of this chapter is 'shock capturing').

17.2 Other Codes for Transonic Flow

From [29] one has the problem of determining $u : R^2 \to R$ such that

$$F(u, u_1, u_2)u_{11} - G(u, u_1, u_2)u_{12} + H(u, u_1, u_2)u_{22} = 0$$

where

$$F(u, u_1, u_2) = a^2 + ((\gamma - 1)/2)(u_0^2 - u_1^2 - u_2^2) - u_1^2$$
$$G(u, u_1, u_2) = -2u_1u_2$$
$$H(u, u_1, u_2) = a^2 + ((\gamma - 1)/2)(u_0^2 - u_1^2 - u_2^2) - u_2^2,$$

a, u_0 being the speed of sound and air velocity at infinity respectively and γ is as in the previous section. For boundary conditions it is required that for each $y \in R$, $\lim_{x\to\infty}(u(x,y) - x) = 0$, $\lim_{x\to\infty}(u_1(x,y) - u_0) = 0$, and $\lim_{x^2+y^2} u_2(x,y) = 0$. Assuming an airfoil as in the previous section, it is also required that the normal velocity component be zero on the object. In [108] Liaw gives a finite element code using Sobolev gradients. In [150] a finite difference code is given for this problem.

17.3 Transonic Flow Plots

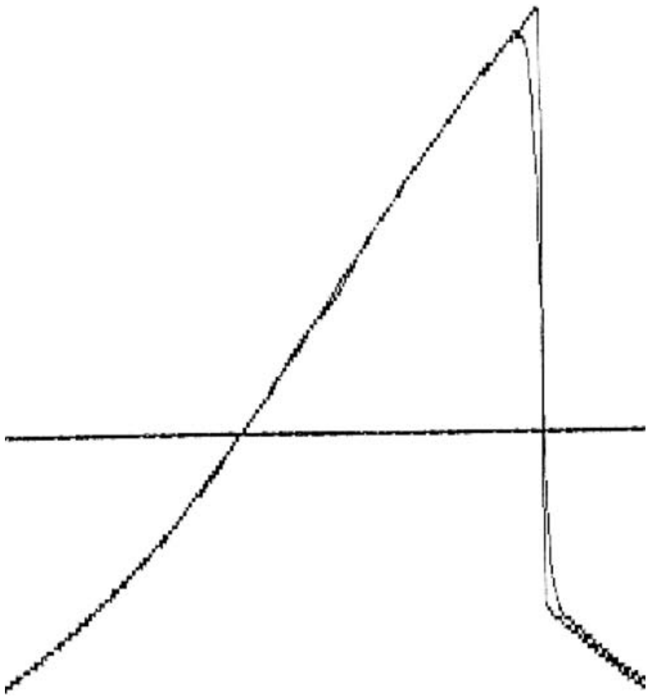

Fig. 17.1 Smeared and Sharp Shocks in Nozzle Problem

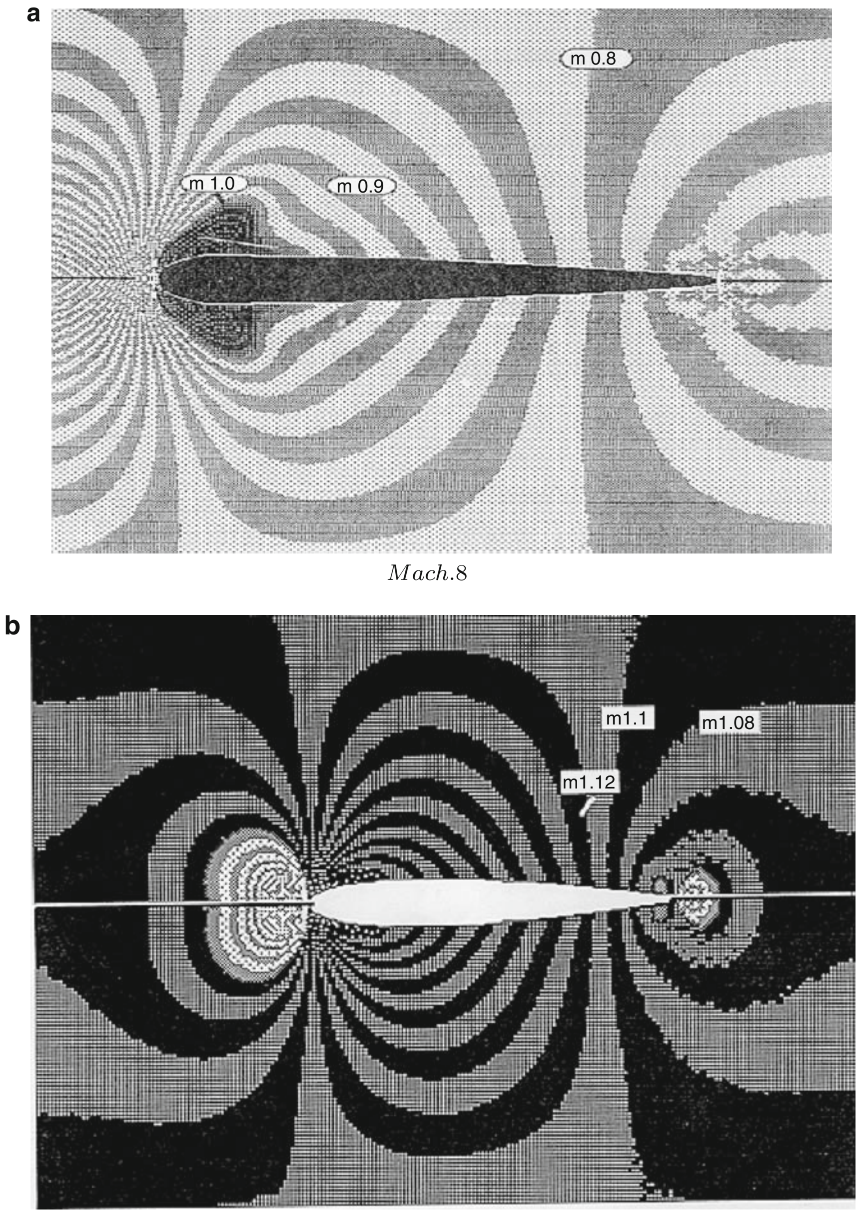

Fig. 17.2 Mach .8 and Mach 1.1 Velocity Contour Plots

Chapter 18
An Alternate Approach to Time-Dependent PDEs

18.1 Introduction

Most of this chapter is take from [168], work by Robert Renka and present writer.

Suppose that X is a Banach space and $F : X \to X$ is such that if $x \in X$, there is a unique function $z : [0, \infty) \to X$ such that

$$z(0) = x, \; z'(t) = F(z(t)), \; t \geq 0. \tag{18.1}$$

For each $\delta > 0$, one has a discrete dynamical system g_δ generated by

$$g_\delta = (I + \delta F(\cdot)). \tag{18.2}$$

There is a general question as to how chaotic behavior of g_δ, for various $\delta > 0$ relate to possible chaotic behavior solutions z to (18.1). Put another way, how do the domains of attraction of (18.1) and (18.2) compare?

As an example, consider continuous Newton's method for finding zeros of a nonconstant complex polynomial p. A trajectory for p is a continuous function $z : R \to C$ such that

$$p(z)' = -p(z), \tag{18.3}$$

or, in a more familiar form,

$$p'(z(t))z'(t) = -p(z(t)), \;\; t \in R.$$

For a discretization, pick $T > 0$ such that $p'(z(t)) \neq 0$ for $t \in [0, T]$, choose a positive integer n and denote $\frac{T}{n}$ by δ. Then Euler's method yields

$$z_k = z_{k-1} - \delta \frac{p(z_{k-1})}{p'(z_{k-1})}, \;\; k = 1, \ldots, n.$$

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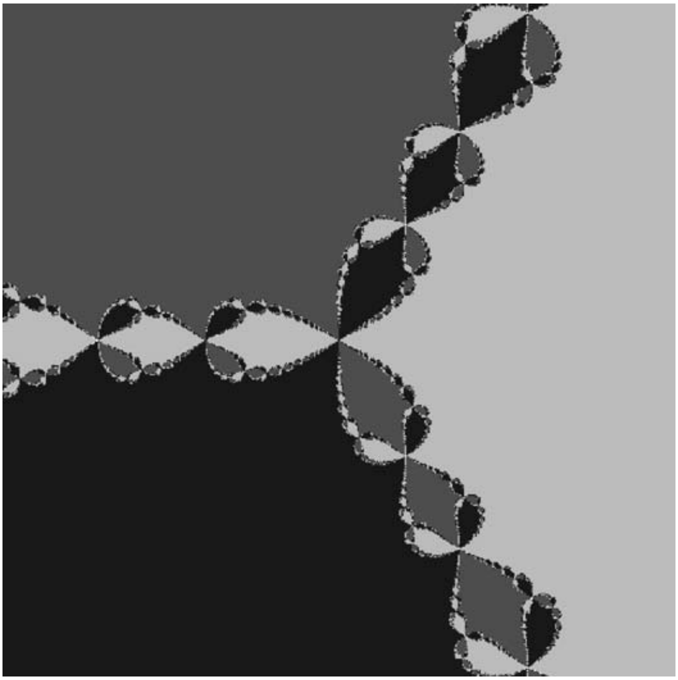


Fig. 18.1 Newton's Method for Cube Roots of 1

This is damped Newton's method (ordinary Newton's method if $\delta = 1$). Now consider the polynomial $p(z) = z^3 - 1$ for $z \in C$. Figure 18.1 depicts the domains of attraction of the three zeros of p for Newton's method ($\delta = 1$); i.e., the color associated with a point in the complex plane is defined by the zero to which the Newton iteration converges when started from that point as initial value. (A background color is assigned to the few points for which the iteration fails to converge to a zero, but these are not noticeable.)

It is well known that the domains of attraction depicted in the figure have fractal boundaries, implying chaotic dynamics. In [169], however, it is proved that no such chaos occurs in the continuous case defined by (18.3). Starting from a point z_0 that does not lie on one of the rays $\theta = \pi/3$, $\theta = -\pi/3$, or $\theta = \pi$, $\lim_{t\to\infty} z(t)$ is the nearest zero to z_0. The only 'chaos' in the differential equation (18.3) is that introduced by discretization.

The above example raises the question of how to separate chaos that is intrinsic to the solution of a differential equation from chaos that arises from numerical approximation. Our primary purpose here is to illustrate a numerical technique that may be helpful in addressing this question. The method is applied to a system of ordinary differential equations, but the method applies equally well to the case of partial differential equations. For example, an important unresolved question is the existence of classical solutions to the incompressible Navier-Stokes equation in three dimensions [63]. The crux of the matter seems to be whether or not there is turbulence and, if so, whether a classical solution ceases to exist at the onset of turbulence. Numerical results have been inconclusive. An alternative approach such as suggested here, might help to resolve this issue.

18.2 Least Squares Method

Suppose m is a positive integer, $T > 0$, and $F : R^m \to R^m$ is continuous. Consider the system of differential equations

$$y'(t) = F(y(t)), \quad t \in [0, T] \tag{18.4}$$

with or without a specified initial value $y(0)$. A discretization of (18.4) is, with $\delta = \frac{T}{n}$ and $Y = (Y_0, Y_1, \ldots, Y_n) \in (R^m)^{n+1}$,

$$Y_k = Y_{k-1} + \delta \frac{F(Y_k) + F(Y_{k-1})}{2}, \quad k = 1, \ldots, n.$$

When applied in a step-by-step manner, this method is referred to in the literature as the trapezoidal method. It is a second-order implicit method with no restriction on the step-size δ required for stability. Rather than single-stepping from an initial value, however, define $\phi : (R^m)^{n+1} \to R$ by

$$\phi(Y) = \frac{1}{2} \sum_{k=1}^{n} \left\| Y_k - Y_{k-1} - \delta \frac{F(Y_k) + F(Y_{k-1})}{2} \right\|^2, \tag{18.5}$$

and find a zero of ϕ by means of a least squares minimization procedure.

A standard method for treating an underdetermined system, such as a damped Newton iteration with a pseudo-inverse Jacobian, works extremely well for this particular problem, requiring very few iterations. However, here is an alternative method that has been shown to work well even when Newton's method fails. Here a Sobolev gradient is used for ϕ which is taken with respect to a metric that emulates the norm associated with the Sobolev space $H^{1,2}([0, T])$, i.e.

$$\|Y\|_S^2 = \sum_{k=1}^{n} \left(\left\| \frac{Y_k + Y_{k-1}}{2} \right\|_{R^m}^2 + \left\| \frac{Y_k - Y_{k-1}}{\delta} \right\|_{R^m}^2 \right), \quad Y = (Y_0, Y_1, \ldots, Y_n) \in (R^m)^{n+1}. \tag{18.6}$$

The Sobolev gradient of ϕ, $\nabla_S \phi$, is defined by

$$(\phi'(Y))h = \langle h, (\nabla_S \phi)(Y) \rangle_S, \quad Y, h \in (R^m)^{n+1},$$

where the inner product is the one associated with $\|\cdot\|_S$ in 18.6). Computationally, $(\nabla_S\phi)(Y)$ is the solution of a linear system in which the right hand side is the ordinary gradient $(\nabla\phi)(Y)$, and the matrix (inverse smoothing operator) is $I + D_1^t D_1$ for the first difference operator D_1. This matrix is tridiagonal and diagonally dominant.

Using this gradient, steepest descent iteration is

$$Y \to Y - \alpha(\nabla_S\phi)(Y), \tag{18.7}$$

with α chosen to minimize

$$\phi(Y - \alpha(\nabla_S\phi)(Y)).$$

A line search is used to approximate α. If a specified value for Y_0 is to be retained, at each step, project the gradient $\nabla_S\phi(Y)$, using the norm (18.6), onto the subspace of vectors that have zero first components (see(8.11)).

18.3 Numerical Results

Our test results were computed using IEEE standard double precision. For a test case the Lorenz equations with standard parameters are used. Define $F : R^3 \to R^3$ by

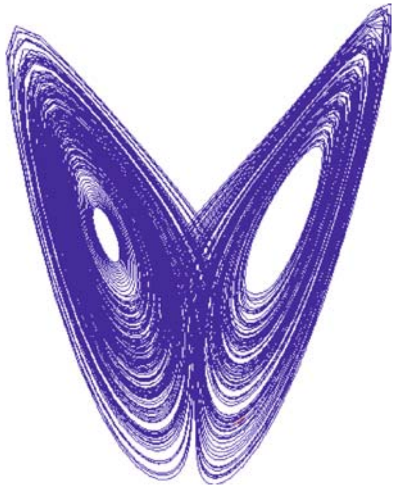
$$F(x, y, z) = \begin{pmatrix} 10(y - x) \\ 28x - y - xz \\ xy - \frac{8}{3}x \end{pmatrix}$$

Use the preceding section to make a numerical least squares formulation on $R^3 \times [0, T]$, for some $T > 0$, of the problem of finding $w : [0, T] \to R^3$ so that

$$w' = F(w).$$

As far as we know all previous numerical approximations to (18.3) over even moderately long time intervals result in the famous 'butterfly' pattern as depicted in Figure 18.2 (see [218]). The least squares method, however, with initial estimate for Y taken to have all $n+1$ components equal to $(10, 12, 14)$ and no enforcement of an end condition, produces a trajectory that follows a smooth curve from a point p_1 to a point p_2 near the critical point $c = (\sqrt{72}, \sqrt{72}, 27)$, spirals in toward the critical point, and then spirals out in approximately the same plane. The curve between p_1 and p_2 is nearly normal to the plane of the spiral with p_2 in the plane and, in some cases, agreeing with c in almost all significant digits (in which cases there is no spiraling in, only spiraling out). This is the case for time interval $T = 800$ with the number of grid points $n = 160{,}000$ corresponding to mesh width

Fig. 18.2 Lorenz Attractor



$\delta = .005$. The first endpoint (initial value) is $p_1 = Y_0 = (10.0094834215091, 7.87724239501250, 26.3369924246729)$, the distance from p_2 to c is about 10^{-15}, and the last point on the curve is (8.8968, 8.9385, 27.453). The radius of the spiral increases very slowly with T.

Using the same (constant) step-size δ and the initial value Y_0 computed by the least squares procedure, we ran the trapezoidal method in step-by-step mode to $T = 800$. The computed trajectory reproduced the curve from p_1 to p_2 but not the spiral. More precisely, the iterates stopped changing after about 500 steps, the final value agreeing with c in all but the last decimal place. We then perturbed the third component of the initial value by 10^{-15} and reran the experiment. This tiny perturbation resulted in the 'butterfly' attractor.

When the nonchaotic orbit (p_1 to p_2) produced by the trapezoidal method was used as initial estimate for the least squares code, with or without prescribed initial value, that orbit was nearly reproduced in a single iteration with a smaller residual than that of the original spiraling solution ($\phi = 8.2\times10^{-27}$ versus $\phi = 4.2\times10^{-25}$). This strongly indicates that spiraling can arise as a numerical artifact in some instances.

As a final test, the least squares code with a prescribed initial value obtained by perturbing Y_0 was run. With the remaining values taken to be initially constant, the method failed to converge, stopping with an uphill search direction. With the computed solution from the trapezoidal method (with perturbed initial value) as initial estimate, the method converged to the butterfly attractor with $\phi = 5.6 \times 10^{-25}$. It is concluded that, as in the case of single-stepping methods, the least squares method with prescribed endpoint value leads to the butterfly attractor when Y_0 is perturbed. This conclusion must be qualified, however, by the fact that the method fails without a reasonably good initial estimate.

Additional test results indicate the existence of at least one non-chaotic orbit for each of the three stationary points. Further testing with different initial estimates for the least squares procedure may reveal additional non-chaotic orbits. Given the extreme sensitivity of these orbits to perturbations in initial values, it is hardly surprising that standard methods fail to produce them. What makes the least squares method work is that at each step, it computes a minimum-norm update to the current approximation, thus producing a solution that is, in some sense, close to the initial estimate, which was taken to be simple constant.

No claim is made for the accuracy of our approximate solutions. In unstable systems such as (18.3) global error cannot be bounded by controlling local discretization error. A computed solution cannot be assured of having any relationship to the actual solution regardless of the computational method. We merely observe the possibility that our method may be capable of picking out solutions that are not accessible to any step-by-step method.

In Section 30.10 there are results using somewhat similar ideas, but for a much more complicated system. the Kuramoto-Sivashinsky equations.

Chapter 19
Foliations and Supplementary Conditions I

For a given system of partial differential equations, what side conditions may be imposed in order to specify a unique solution? For various classes of elliptic, parabolic or hyperbolic equations there are, of course, well established criteria in terms of boundary conditions. For many systems, however, there is some mystery concerning characterization of the set of all solutions to the system.

19.1 A Foliation Theorem

This section is taken largely from [163]. Suppose that each of H and K is a Hilbert space and F is a $C^{(3)}$ function from $H \to K$. Define

$$\phi : H \to R$$

by

$$\phi(x) = \frac{1}{2}\|F(x)\|_K^2, \ x \in H$$

and note that

$$\phi'(x)h = \langle F'(x)h, F(x)\rangle_K = \langle h, F'(x)^* F(x)\rangle_H, \ x, h \in H \tag{19.1}$$

where $F'(x)^* \in L(K, H)$ is the Hilbert space adjoint of $F'(x), x \in H$. In view of (19.1), take $F'(x)^*F(x)$ to be $(\nabla\phi)(x)$, the gradient of ϕ at x.

By Theorem 4.1 there is a unique function

$$z : [0, \infty) \times H \to H$$

such that

$$z(0, x) = x, \ z_1(t, x) = -(\nabla\phi)(z(t, x)), \ t \geq 0, \ x \in H \tag{19.2}$$

where the subscript in (19.2) indicates the partial derivative of z in its first argument.

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_19,

In this chapter there are the following standing assumptions on F : If $r > 0$, there is $c > 0$ such that

$$\|F'(x)^* g\|_H \geq c\|g\|_K,\ \|x\| < r,\ g \in K \tag{19.3}$$

and if

$$x \in H, z(0,x) = x, z_1(t,x) = -(\nabla\phi)(z(t,x))t > 0,$$

then

$$\{z(t,x) : t \geq 0\}\ \text{ is bounded.}$$

Using Theorem 4.4, if $x \in H$, then

$$u = \lim_{t\to\infty} z(t,x),\ \text{exists and } F(u) = 0. \tag{19.4}$$

Define $G : H \to H$ so that if $x \in H$ then $G(x) = u, u$ as in (19.4). Denote by Q the collection of all $g \in C^{(1)}(H,R)$ so that

$$g'(x)(\nabla\phi)(x) = 0,\ x \in H.$$

Theorem 19.1. *(a) G' exists, has range in $L(H,H)$ and*

$$(b)\quad G^{-1}(G(x)) = \cap_{g\in Q}\ g^{-1}(g(x)),\ x \in H.$$

A proof depends on a number of lemmas to follow.

Lemma 19.2. *Under the standing hypothesis suppose $x \in H$ and*

$$Q = \{z(t,x), t \geq 0\} \cup \{G(x)\}.$$

There are $\gamma, M, r, T > 0$ so that if

$$Q_\gamma = \cup_{w\in Q} B_\gamma(w),$$

then

$$|(\nabla\phi)'(w)| \leq M,\ |(\nabla\phi)''(w)| \leq\ M, w \in Q$$

and if $y \in H$, $\|y - x\|_H < r$, then

$$[z(t,y), z(t,x)] \subset Q_\gamma,\ t \geq 0 \text{ and } [\mathrm{z(t,y), G(y)}] \subset \mathrm{Q}_{\gamma,}\ \mathrm{t} \geq \mathrm{T}.$$

For $a, b \in H$, $[a,b] = \{ta + (1-t)b : 0 \leq t \leq 1\}$ and for $w \in H$, $|(\nabla\phi)'(w)|$, $|(\nabla\phi)''(w)|$ denote the norms of $(\nabla\phi)'(w)$, $(\nabla\phi)''(w)$ as linear and bilinear functions on $H \to H$ respectively:

$$|(\nabla\phi)'(w)| = \sup_{h\in H, \|h\|_H=1} |(\nabla\phi)'(w)h|$$

$$|(\nabla\phi)''(w)| = \sup_{h,k\in H, \|h\|_H=1, \|k\|_H=1} |(\nabla\phi)''(w)(h,k)|.$$

Proof. Since Q is compact and both $(\nabla\phi)', (\nabla\phi)''$ are continuous on H, there is $M > 0$ and an open subset α of H containing Q so that

$$|(\nabla\phi)'(w)|, |(\nabla\phi)''(w)| < M,\ w \in \alpha.$$

Pick $\gamma > 0$ such that $Q_\gamma \subset \alpha$. Then the first part of the conclusion clearly holds.

Note that Q_γ is bounded. Denote by c a positive number so that

$$\|F'(w)^* g\|_H \geq c\|g\|_K,\ g \in K,\ w \in Q_\gamma.$$

Pick $T > 0$ so that $\|z(T,x) - G(x)\|_H < \gamma/4$ and $\|F(z(T,x))\|_K < c\gamma/4$ (this is possible since $\lim_{t\to\infty} F(z(t,x)) = F(u) = 0$). Pick $v > 0$ such that $v \cdot \exp(TM) < \gamma/4$. Suppose

$$y \in B_v(x) \ \ (= \{w \in H : \|w - x\|_H < v)\}.$$

Then

$$z(t,y) - z(t,x) = y - x - \int_0^t ((\nabla\phi)(z(s,y)) - (\nabla\phi)(z(s.x)))\, ds$$

and so

$$z(t,y) - z(t,x) = y - x$$
$$- \int_0^t \int_0^1 [((\nabla\phi)'((1-\tau)z(s,x) + \tau z(s,y)))\, d\tau](z(s,y) - z(s,x))\, ds,\ t \geq 0.$$

Hence there is $T_1 > 0$ such that $[z(s,y), z(s,x)] \subset Q_\gamma$, $0 \leq s \leq T_1$, and so

$$|\int_0^1 ((\nabla\phi)'((1-\tau)z(s,x) + \tau z(s,y)))\, d\tau| \leq M$$

and

$$\|z(t,y) - z(t,x)\|_H \leq \|y - x\|_H + M\int_0^t \|z(s,y) - z(s,x)\|_H ds,\ 0 \leq s \leq T_1.$$

But this implies that

$$\|z(t,y) - z(t,x)\|_H \leq \|y - x\|_H \exp(tM) < v \cdot \exp(tM)$$
$$\leq v \cdot \exp(T_1 M) < \gamma, \|y - x\|_H < r$$

and so

$$[z(t,y), z(t,x)] \subset Q_\gamma, \|y-x\|_H < v,\ 0 \le t \le T_1.$$

Supposing that the largest such T_1 is less than T, there is a contradiction and so

$$[z(t,y), z(t,x)] \subset Q_\gamma, 0 \le t \le T,\ \|y-x\|_H < r.$$

Now choose $r > 0$ such that $r \le v$ and such that if $\|y-x\|_H < r$, then

$$\|F(y)\|_K \le 2\|F(x)\|_K, \|z(T,y) - z(T,x)\|_H < \gamma/4$$

and

$$\|F(z(T,y)) - F(z(T,x))\|_K < c\gamma/4.$$

Hence for $\|y-x\|_H < r$,

$$\|z(T,y) - G(x)\|_H \le \|z(T,y) - z(T,x)\|_H + \|z(T,x) - G(x)\|_H < \gamma/2$$

and

$$\|F(z(T,y))\|_K \le \|F(z(T,y)) - F(z(T,x))\|_K + \|F(z(T,x))\|_K < c\gamma/2.$$

According to Theorem 4.12 it must be that

$$\|z(t,y) - z(T,y)\|_H < \gamma/2,\ t \ge T$$

and so

$$\|G(y) - z(T,y)\|_H \le \gamma/2,$$

since $G(y) = \lim_{t\to\infty} z(t,y)$. Note also that Theorem 4.12 gives that

$$\|z(t,x) - z(T,x)\|_H < \gamma/2,\ t \ge T$$

and so the convex hull of

$$G(x), G(y), \{z(t,x) : t \ge T\}, \{z(t,y) : t \ge T\}$$

is a subset of $B_\gamma(G(x)) \subset \alpha$. This gives us the second part of the conclusion since

$$[z(t,y), z(t,x)] \subset Q_\gamma,\ 0 \le t \le T.$$

□

Lemma 19.3. *Suppose $B \in L(H,K)$, $c > 0$ and*

$$\|B^* g\|_H \ge c\|g\|_K,\ g \in K. \tag{19.5}$$

Then

$$|\exp(-tB^*B) - (I - B^*(BB^*)^{-1}B)| \leq \exp(-tc^2),\ t \geq 0.$$

Note that the spectral theorem (cf [204]) gives that $\exp(-tB^*B)$ converges pointwise on H to $(I - B^*(BB^*)^{-1}B)$, the orthogonal projection of H onto $N(B)$, as $t \to \infty$. What Lemma 19.3 gives is exponential convergence in operator norm.

Proof. First note that (19.5) is sufficient for

$$(BB^*)^{-1}$$

to exist and belong to $L(K, K)$. Note next the formula

$$\exp(-tB^*B) = I - B^*(BB^*)^{-1}B + B^*(BB^*)^{-1}\exp(-tBB^*)B \qquad (19.6)$$

which is established by expanding $\exp(-tBB^*)$ in its power series and collecting terms, $t \geq 0$. Note also that

$$B^*(BB^*)^{-1}\exp(-tBB^*)B = B^*(BB^*)^{-1/2}\exp(-tBB^*)(BB^*)^{-1/2}B$$

and that

$$|B^*(BB^*)^{-1/2}| = |(BB^*)^{-1/2}B| \leq 1$$

and hence

$$|B^*(BB^*)^{-1}\exp(-tBB^*)B| \leq |\exp(-tBB^*)|.$$

Now denote by ξ a spectral family for BB^*. Since

$$\langle BB^*g, g\rangle_K = \|B^*g\|_K^2 \geq c^2\|g\|_K^2,\ g \in K$$

it follows that c^2 is a lower bound to the numerical range of BB^*. Denote by b the least upper bound to the numerical range of BB^*. Then

$$BB^* = \int_{c^2}^{b} \lambda\, d\xi(\lambda)$$

and

$$\exp(-tBB^*) = \int_{c^2}^{b} \exp(-t\lambda)d\xi(\lambda),\ t \geq 0.$$

But this implies that $|\exp(-tBB^*)| \leq \exp(-tc^2)$, $t \geq 0$. This fact together with (19.5),(19.6) give the conclusion to the lemma. □

Lemma 19.4. *Suppose x, γ, M, r, T, c are as in Lemma 19.2. If $\|x - w\| < r$, then*

$$\|z(t, w) - G(w)\| \leq M_2 \exp(-tc^2),\ t \geq 0$$

where

$$M_2 = 2^{-1/2}\|F(x)\|/(1 - \exp(-c^2)).$$

Proof. This follows from the argument for Theorem 4.4. □

From ([66], Theorem (3.10.5)), $z_2(t, w)$ exists for all $t \geq 0, w \in H$ and that z_2 is continuous. Furthermore if $Y(t, w) = z_2(t, w),\ t \geq 0,\ w \in H$, then

$$Y(0, w) = I, Y_1(t, w) = -(\nabla\phi)'(z(t, w))Y(t, w),\ t \geq 0,\ w \in H.$$

Consult [66] for background on various techniques with differential inequalities used in this chapter.

Lemma 19.5. *Suppose x, γ, M, r, T, c are as in Lemma 19.2 and $\epsilon > 0$. There is $M_0 > 0$ so that if $t > s > M_0$ and $\|w - x\|_H < r$, then*

$$|Y(t, w) - Y(s, w)| < \epsilon.$$

Proof. First note that if $\|w - x\|_H < r$ then

$$|Y(t, w)| \leq \exp(Mt),\ t \geq 0 \ \text{ since}$$

$$Y(t, w) = I - \int_0^t (\nabla\phi)'(z(s, w))Y(s, w)\, ds,\ t \geq 0 \tag{19.7}$$

and $|(\nabla\phi)'(z(s, w))| \leq M,\ 0 \leq s$. In particular,

$$|Y(T, w)| \leq \exp(MT),\ \|w - x\|_H < r.$$

Suppose that $t > s \geq T$ and $\delta = t - s$. Then

$$|Y(t, w) - Y(s, w)| = \lim_{n\to\infty} |(\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(z(s + (k-1)\delta/n, w))))Y(s)|$$

(This formula expresses the fact that the Cauchy polygon methods works for solving (19.7) on the interval $[s, t]$). For n a positive integer and $\|w - x\|_H < r$,

$$\begin{aligned}
&|(\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(z(s + (k-1)\delta/n, w))))Y(s, w)| \\
&\quad \leq |(\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(G(w))))Y(s, w)| \\
&\quad + |(\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(z(s + (k-1)\delta/n, w))))Y(s, w) \\
&\quad - (\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(G(w))))Y(s, w)|
\end{aligned}$$

Now by Lemma 19.3,

$$|(\Pi_{k=1}^n (I - (\delta/n)(\nabla\phi)'(G(w))))Y(s, w)| \leq \exp(-c^2 s)|Y(s, w)|.$$

Define

$$A_k = I - (\delta/n)(\nabla\phi)'(z(s + (k-1)\delta/n, w))$$

and

$$B_k = I - (\delta/n)(\nabla\phi)'(G(w)),$$

$k = 1, 2, ..., n$, and denote $Y(s, w)$ by W. By induction,

$$|(\Pi_{k=1}^n A_k)W - (\Pi_{k=1}^n B_k)W| \le \sum_{k=1}^n |A_n \cdots A_{k+1}(A_k - B_k)B_{k-1} \cdots B_1 W|.$$

Now

$$\begin{aligned}
|A_j| &\le |I - (\delta/n)(\nabla\phi)'(z(G(w)))| \\
&\quad + (\delta/n)|(\nabla\phi)'(G(w)) - (\nabla\phi)'(z(s + (j-1)\delta/n, w))| \\
&\le 1 + (\delta/n)M|(\nabla\phi)'(G(w)) - (\nabla\phi)'(z(s + (j-1)\delta/n, w))| \\
&\le 1 + (\delta/n)(\int_0^1 |(\nabla\phi)''((1-\tau)z(s + (j-1)\delta/n, w) + \tau G(w)|dr) \\
&\times \|G(y) - z(s + (j-1)\delta/n, w)\|_H \\
&\le 1 + (\delta/n)M\|G(y) - z(s + (j-1)\delta/n, w)\|_H \\
&\le 1 + (\delta/n)MM_2 \exp(-c^2(s + (j-1)\delta/n) \\
&= 1 + (\delta/n)M_3 \exp(-c^2 s)(\exp(-c^2\delta/n))^{j-1},
\end{aligned}$$

$j = 1, ..., n$. Note that $|B_j| \le 1, j = 1, ..., n$. Note also that

$$|A_n \cdots A_{k+1}| \le |A_n| \cdots |A_{k+1}| \tag{19.8}$$

$$\le \Pi_{j=k+1}^n (1 + (\delta/n)M_3 \exp(-c^2 s)(\exp(-c^2\delta/n))^{j-1})$$

$$\le \Pi_{j=k+1}^n \exp((\delta/n)M_3 \exp(-c^2 s)(\exp(-c^2\delta/n))^{j-1})$$

$$\le \exp(M_3 \exp(-c^2 s)(\delta/n) \sum_{j=k+1}^n (\exp(-c^2\delta/n))^{j-1})$$

$$\le \exp(M_3 \exp(-c^2 s)(\delta/n)/(1 - \exp(-c^2\delta/n)))$$

$$\le \exp(M_4 \exp(-c^2 s))$$

so long as $\delta/n \le 1$, where $M_4 = M_3 \sup_{\beta\in(0,1]} \beta/(1 - \exp(-c^2\beta))$ and $M_3 = MM_2$. Note that

$$\begin{aligned}
|A_k - B_k| &= (\delta/n)|(\nabla\phi)'(z(s + (j-1)\delta/n, w)) - (\nabla\phi)'(G(w))| \\
&= (\delta/n)|(\int_0^1 (\nabla\phi)''((1-\tau)z(s + (j-1)\delta/n, w) + \tau G(w))\, d\tau
\end{aligned}$$

$$\begin{aligned}&(z(s+(j-1)\delta/n,w)-G(w))|\\&\leq (\delta/n)M|(z(s+(j-1)\delta/n,w)-G(w))|\\&\leq (\delta/n)MM_2\exp(-c^2s)(\exp(-c^2\delta/n)^{j-1}),\ k=1,...,n,\end{aligned}$$

and so using the above and (19.8),

$$\begin{aligned}|(\Pi_{k=1}^n A_k)W-(\Pi_{k=1}^n B_k)W| &\leq \sum_{k=1}^n \exp(M_4\exp(-c^2s))|A_k-B_k||W|\\&\leq \exp(M_4\exp(-c^2s))MM_2\exp(-c^2s)\\&\quad\times\sum_{k=1}^n \exp(-c^2\delta/n)^{k-1})|W|\\&\leq \exp(M_4\exp(-c^2s))\exp(-c^2s))M_4|W|.\end{aligned}$$

Thus

$$\begin{aligned}&|(\Pi_{k=1}^n(I-(\delta/n)(\nabla\phi)'(z(s+(k-1)\delta/n,w))))Y(s,w)|\\&\leq |(\Pi_{k=1}^n(I-(\delta/n)(\nabla\phi)'(G(w))))Y(s,w)|\\&+\exp(M_4\exp(-c^2s))\exp(-c^2s)M_4|Y(s,w)|\end{aligned}$$

Taking the limit of both sides of the above as $n\to\infty$,

$$|Y(t,w)-Y(s,w)|\leq \exp(-c^2s)|Y(s,w)|(1+\exp(M_4\exp(-c^2s))M_4)$$

$0<T\leq s<t$. Taking for the moment $s=T$ the above yields

$$|Y(t,w)-Y(T,w)|\leq \exp(-c^2T)|Y(T,w)|(1+\exp(M_4\exp(-c^2T))M_4).$$

Note $\{|Y(T,w)|,\ \|y-x\|_H<r\}$ is bounded, say by $M_5>0$. Hence

$$|Y(t,w)-Y(T,w)|\leq$$

$$\exp(-c^2s)M_5(1+\exp(M_4\exp(-c^2T))M_4),\ t>s\geq T,\ \|w-x\|_H<r,$$

and so the conclusion follows. □

Denote by U the function with domain $B_r(x)$ to which $\{Y(t,\cdot)\}_{t\geq 0}$ converges uniformly on $B_r(x)$. Note that $U:B_r(x)\to L(H,H)$. and U is continuous.

Lemma 19.6. *Suppose that $x\in H$, $r>0$, each of $v_1,v_2,...$ is a continuous function from $B_r(x)\to H$, q is a continuous function from H to $L(H,H)$ which is the uniform limit of $v_1',v_2',....$ on $B_r(x)$. Then q is continuous and*

$$v'(y)=q(y),\|y-x\|_H<r.$$

Proof. Suppose $y \in B_r(x)$, $h \in H$, $h \neq 0$ and $y + h \in B_r(x)$. Then

$$\int_0^1 q(y+sh)h\ ds = \lim_{n\to\infty} \int_0^1 v_n'(y+sh)h\ ds$$

$$= \lim_{n\to\infty} (v_n(y+h) - v_n(y)) = v(y+h) - v(y).$$

Thus

$$\|v(y+h) - v(y) - q(y)h\|_H / \|h\|_H = \| \int_0^1 q(y+sh)h - q(y)h)ds\|$$

$$\leq \int_0^1 |q(y+sh) - q(y)|ds \to 0$$

as $\|h\| \to 0$. Thus v is Fréchet differentiable at each $y \in B_r(x)$ and $v'(y) = g(y)$, $y \in B_r(x)$. □

Proof. To prove Theorem 19.1, note that Lemmas 19.4,19.5,19.6 give the first conclusion. To establish the second conclusion, suppose that $g \in Q$. Suppose $x \in H$ and $\beta(t) = g(z(t,x)),\ t \geq 0$. Then

$$\beta'(t) = g'(z(t,x))z_1(t,x) = -g'(z(t,x))(\nabla\phi)(z(t,x)),\ t \geq 0.$$

Thus β is constant on

$$R_x = \{z(t,x) : t \geq 0\} \cup \{G(x)\}.$$

But if

$$y \in \overline{G^{-1}(G(x))} \text{ then } g(\{z(t,y) : t \geq 0\} \cup \{G(y)\})$$

must also be in $G^{-1}(G(x))$ since $G(y) = G(x)$. Thus $G^{-1}(G(x))$ is a subset of the level set $g^{-1}(g(x))$ of g. Therefore,

$$G^{-1}(G(x)) \subset \cap_{g\in Q} g^{-1}(g(x)).$$

Suppose now that

$$x \in H, y \in \cap_{g\in Q} g^{-1}(g(x)) \text{ and } y \notin G^{-1}(G(x)).$$

Denote by f a member of H^* so that $f(G(x)) \neq f(G(y))$. Define $p : H \to R$ by $p(w) = f(G(w)), w \in H$. Then $p'(w)h = f'(G(w))G'(w)h$ and so

$$p'(w)(\nabla\phi)(w) = fG'(w)(\nabla\phi)(w) = 0,$$

$w \in H$, and hence $p \in Q$, a contradiction since

$$y \in \cap_{q \in Q} g^{-1}(g(x)) \text{ and } p \in Q$$

together imply that $p(y) = p(x)$. Thus

$$G^{-1}(G(x)) \supset \cap_{q \in Q} g^{-1}(g(x))$$

and the second part of the theorem is established. □

This section ends with an example.

19.2 A Linear Example

Example. Take H to be the Sobolev space $H^{1,2}([0,1]), K = L_2([0,1])$,

$$F(y) = y' - y,\ y \in H.$$

It is claimed that the corresponding function G is specified by

$$(G(y))(t) = \exp(t)(y(1)e - y(0))/(e^2 - 1),\ t \in [0,1],\ y \in H. \tag{19.9}$$

In this case

$$G^{-1}(G(x)) = \{w \in H : w(1)e - w(0) = y(1)e - y(0)\}.$$

This may be observed by noting that since F is linear,

$$(\nabla\phi)(y) = F^*Fy,\ y \in H.$$

The equation

$$z(0) = y \in H, z'(t) = -F^*Fz(t),\ t \geq 0$$

has the solution

$$z(t) = \exp(-tF^*F)y,\ t \geq 0.$$

But $\exp(-tF^*F)y$ converges to

$$(I - F^*(FF^*)^{-1}F)y,$$

the orthogonal projection of y onto $N(F)$, *i.e.*, the solution $w \in H$ to $F(w) = 0$ that is nearest (in H) to y. A little calculation shows that this nearest point is given by $G(y)$ in (19.9). The quantity

$$(y(1)e - y(0))/(e^2 - 1)$$

provides an invariant for steepest descent for F relative to the Sobolev metric $H^{1,2}([0,1])$. Similar reasoning applies to all cases in which F is linear but invariants are naturally much harder to exhibit for more complicated functions F. In summary, for F linear, the corresponding function G is just the orthogonal projection of H onto $N(F)$. In general G is a projection on H in the sense that it is an idempotent transformation. It is hoped that a study of these idempotents in increasingly involved cases will give information about 'boundary conditions' for significant classes of partial differential equations.

Chapter 20
Foliations and Supplementary Conditions II

This chapter gives a another development on a general approach to the 'boundary condition' problem. In particular, the strong condition (19.3), which implies that a gradient inequality be satisfied on any bounded set, is not required. First are introduced some ideas from the theory of nonlinear semigroups using the approach in [52].

20.1 Semigroups on a Metric Space

- X : complete separable metric space (Polish space).
- $T : [0, \infty) \to$ set of transformations from X to X.
- $T(0)$: identity transformation on X .
- $T(t)T(s) = T(t+s),\ t, s \geq 0$ (indicated product is composition).

Such a semigroup T is called jointly continuous provided:

- If $g : [0, \infty) \times X \to X$ is defined by $g(t, x) = T(t)x, t \geq 0, x \in X$, then g is continuous.

Here is some more notation:

- $CB(X)$: Banach space of bounded continuous functions $X \to R$.
- $SG(X)$: all jointly continuous semigroups on X.
- If $T \in SG(X)$, Lie generator A of T is:

$$\{(f, g) \in CB(X)^2 : g(x) = \lim_{t \to 0+} \frac{1}{t}(f(T(t)x) - f(x)),\ x \in X\}.$$

- $\{f_n)\}_{n=1}^{\infty}$ $\beta-$converges to $f \in CB(X)$ if it is uniformly bounded and converges uniformly to f on compact subsets of X.

$LG(X)$ denotes the collection of all linear transformations A which have domain and range in $CB(X)$ and have the following four properties:

- A is a derivation (if $f, g \in D(A)$ then the product $fg \in D(A)$ and A(fg) = fAg + gAf).

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- $D(A)$ is dense in $CB(X)$ in the sense of $\beta-$convergence.
- For each $\lambda > 0$, $(I - \lambda A)$ has a norm-nonexpansive inverse with domain all of $CB(X)$.
- If $\eta > 0$, then the collection

$$\{(I - \frac{\lambda}{n}A)^{-n},\ 0 < \lambda \leq \eta,\ n = 1, 2, \dots\}$$

is $\beta-$ equicontinuous.

The following, from [52], is the fundamental result for this kind of semigroup. See [52] for an argument.

Theorem 20.1. *If $A \in LG(X)$ there is a unique $T \in SG(X)$ with Lie generator A and*

$$f(T(t)x) = \lim_{n\to\infty}((I - \frac{t}{n}A)^{-n}f)(x),\ x \in X,\ t \geq 0,\ f \in CB(X). \quad (20.1)$$

Conversely, if $T \in SG(X)$ and A its Lie generator, then $A \in LG(X)$.

This theorem, due to J.R. Dorroh and the present writer, is the end result of a three decade quest for a suitable generalization of linear semigroup theory (cf [73, 204]) to significant nonlinear cases. The quest for a long time was an attempt to generalize existing linear theory to a nonlinear case. Some hold that [134] was the opening work in this direction. It turns out that Theorem 20.1 is more an *application* of linear theory. The notion of generator used, the Lie generator indicated above, is defined by differentiation that is in the spirit of Gauss, Riemann and Lie.

Following is an application of this result to the problem of specification of supplementary conditions for partial differential equations.

20.2 Application: Supplementary Condition Problem

Denote by

- X a separable Banach space.
- $\phi : X \to [0, \infty)$ a C^2 function.
- T the semigroup on X so that if $s \geq 0$ and $x \in X$, then $T(s)x = z(s)$, where $z(0) = x,\ z'(t) = -(\nabla\phi)(z(t)),\ t \geq 0$.

Theorem 20.2. *Suppose*

- *G is a continuous function on all of X so that if $x \in X$ then $G(x) = \lim_{t\to\infty} T(t)x$.*
- *A is the Lie generator of T.*

Then

$$G^{-1}(G(x)) = \cap_{g \in N(A)} g^{-1}(g(x)),\ x \in X. \tag{20.2}$$

Proof. Suppose that each of $x, y \in X$ and

$$y \in \cap_{g \in N(A)} g^{-1}(g(x)) \text{ but } y \notin G^{-1}(G(x)).$$

Then $G(y) \neq G(x)$. Pick $r > 0$ so that $\|G(x) - G(y)\|_X > r$ and denote by k the element of $CB(X)$ so that if $p \in X$, then

$$k(p) = \begin{cases} r - \|G(x) - p\|_X, & \text{if } \|G(x) - p\|_X \leq r \\ 0, & \text{if } \|G(x) - p\|_X > r. \end{cases}$$

Note that $f = k \circ G \in N(A)$ since G, k are continuous, G is constant on trajectories of T and k is bounded. But

$$f(x) = k(G(x)) \neq k(G(y)) = f(y),$$

a contradiction since

$$y \in \cap_{g \in N(A)} g^{-1}(g(x)) \text{ and } f \in N(A).$$

Now suppose that $x \in H,\ y \in G^{-1}(G(x))$ and $f \in N(A)$. Denote $G(x) = G(y)$ by u. Then if $t \geq 0, w \in X$,

$$0 = (Af)(T(t)w) = \lim_{h \to 0+} \frac{1}{h} f(T(h)(T(t)w)) - f(T(t)w)) = f(T(\cdot)x)'(t).$$

The above holds since a function on $[0, \infty)$ which has a continuous right derivative on all of $[0, \infty)$ is actually differentiable. Thus, each of

$$f(T(\cdot)w)),\ w = x, y$$

is constant, necessarily at u since

$$\lim_{t \to \infty} T(t)x = G(x) = u = G(y) = \lim_{t \to \infty} T(t)y,$$

Thus,

$$f(y) = f(T(0)y) = u = f(T(0)x) = f(x),$$

and so

$$y \in f^{-1}(f(x)).$$

Since f was an arbitrary member of $N(A)$,

$$y \in \cap_{g \in N(A)} g^{-1}(g(x))$$

and the argument is finished. □

The sets on the left side of (20.2) are equivalence classes, each containing precisely one critical point of ϕ. These equivalence classes give a foliation of X. If for a given function ϕ this foliation is understood, then one understands the set of all critical points of ϕ, in applications the set of all solutions to some system of partial differential equations. (20.2) gives a characterization of this foliation. If the null space of A is somehow understood in a given instance, then this theorem gives in turn an understanding of the corresponding foliation. It is pointed out that even when the critical points of ϕ correspond to the set of all solutions to some system of nonlinear partial differential equations, A is still a linear transformation but it nevertheless carries full information about T due to (20.1). Thus, in principle, the task of characterizing the set of all solutions to many systems of partial differential equations has become a problem in linear analysis (not a particularly easy problem, to be sure). An interested reader who grasps Theorem 20.2 can easily construct a version in which X is some closed subset of H. A reader might see how the Tricomi equation in Chapter 15 fits in with the present chapter.

20.3 Computational Fantasy

Can useful information come from considerations in the preceding section? Consider a problem as in Chapter 17, specifically the two dimensional transonic flow problem. For such problems solution type depends on nonlinearity and so choice of boundary or supplementary conditions may be even more of a mystery than for Tricomi's equation. Here is an outline of a possible computational attack on the supplementary condition problems for this type of problem. A Hilbert space setting is assumed.

Suppose one has a problem on a three dimensional region Ω for which one doesn't have boundary conditions which are sufficient to give a unique solution to the problem, that is a critical point of an appropriate functional ϕ. Such a region might require n^3 grid points with maybe $n = 100$. First decide upon an appropriate discrete version of a space X as in the previous section. Then consider a discrete version of the corresponding space $CB(X)$ as well as a discrete version of the Lie generator A. A next task is a determination of a numerical rendering of $N(A)$, the null space of A. Pick x in the discrete version of X and a member g of our discrete version of $N(A)$ and compute all y so that

$$y \in g^{-1}(g(x)), \text{ i.e., } g(y) = g(x). \tag{20.3}$$

Then seek a representation of all sets so obtained. Then take the intersection of all these sets. This intersection would be one leaf in the desired approximation to a foliation. Once a significant number of such leaves are obtained, one would have a collection which is one-to-one with a large collection of numerical approximations to critical points of the underlying functional ϕ. These seem to be very large tasks: computing functions g, taking level sets using (20.3), then computing intersections corresponding to these level sets, and finally organizing the collection of level sets so obtained to get an idea of the set of all critical points of ϕ.

Such a computation seems challenging computationally and may be beyond present machines, but the trend in the development of ever larger and faster machines may eventually allow such a computation. At least as promising is the prospect into new insights which would reduce the complexity of what is outlined above.

Chapter 21
Some Related Iterative Methods for Differential Equations

This chapter describes two developments which had considerable influence on the theory of Sobolev gradients. They both deal with projections. As a point of departure, we indicate a result of von Neumann ([78, 223]).

Theorem 21.1. *Suppose H is a Hilbert space and each of P and L is an orthogonal projection on H. If Q denotes the orthogonal projection of H onto $R(P) \cap R(L)$, then*

$$Qx = \lim_{n\to\infty} (PLP)^n x,\ x \in H. \tag{21.1}$$

If $T, S \in L(H,H)$, and are symmetric, then $S \leq T$ means

$$\langle Sx, x\rangle \leq \langle Tx, x\rangle,\ x\ inH.$$

Proof. (Indication) First note that $\{(PLP)^n\}_{n=1}^{\infty}$ is a non-increasing sequence of symmetric members of $L(H,H)$ which is bounded below (each term is non-negative) and hence $\{(PLP)^n\}_{n=1}^{\infty}$ converges pointwise on H to a non-negative symmetric member Q of H which is idempotent and which commutes with both P and L. Since Q is also fixed on $R(P), R(L)$ it must be the required orthogonal projection. □

How might this applied to differential equations is illustrated first by a simple example.

Example 15.1. Suppose $H = L_2([0,1])^2, P$ is the orthogonal projection of H onto

$$\{\binom{u}{u'}\} : u \in H^{1,2}([0,1])\}$$

and L is the orthogonal projection of H onto

$$\{\binom{u}{u} : u \in L_2([0,1])\}.$$

Then

$$R(P) \cap R(L) = \{\binom{u}{u'} : u \in H^{1,2}([0,1]),\ u' = u\}.$$

Thus $R(P) \cap R(L)$ essentially yields solutions u to $u' = u$.

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The above example is so simple that a somewhat more complicated one might shed more light.

Example 15.2. Suppose that each of a, b, c, d is a continuous real-valued function on $[0, 1]$ and denote by L the orthogonal projection of $H = L_2([0, 1])^4$ onto

$$\{(u, au + bv, v, cu + dv) : u, v \in L_2([0, 1])\}. \tag{21.2}$$

Denote by P the orthogonal projection of H onto

$$\{(u, u', v, v') : u, v \in H^{1,2}([0, 1])\} \tag{21.3}$$

Then

$$(u, f, v, g) \in R(P) \cap R(L)$$

if and only if

$$f = u', g = v',\ f = au + bv, g = cu + dv,$$

that is, the system

$$u' = au + bv,\ \ v' = cu + dv \tag{21.4}$$

is satisfied.

In a sense (21.4) is split into an algebraic part represented by (21.2) and an analytical part (i.e., a part in which derivatives occur) (21.3). Then $R(P) \cap R(L)$ gives us all solutions to (21.4). One may see that the iteration (21.1) provides a constructive way to calculate a solution since P is presented constructively. As to a construction for L observe that if

$$t \in [0, 1],\ \alpha = a(t),\ \beta = b(t),\ \gamma = c(t),\ \delta = d(t),\ p, q, r, s \in R$$

then the minimum (x, y) to

$$\|(p, q, r, s) - (x, \alpha x + \beta y, y, \gamma x + \delta y)\| \tag{21.5}$$

is given by the unique solution (x, y) to

$$(1 + \alpha^2 + \gamma^2)x + (\alpha\beta + \gamma\delta)y = p + \alpha q + \gamma s$$
$$(\alpha\beta + \gamma\delta)x + (1 + \beta^2 + \delta^2)y = r + \beta q + \delta s.$$

It is remarked that appropriate boundary conditions could be imposed using the ideas of Chapter 6.

From [145] there is a nonlinear generalization of (21.1). Suppose that H is a Hilbert space, P is an orthogonal projection on H and Γ is a strongly continuous function from H to

$$B_1(H) = \{T \in L(H, H) : T^* = T, 0 \le \langle Tx, x\rangle \le \|x\|^2,\ x \in H\}.$$

For T any non-negative symmetric member of $L(H,H), T^{1/2}$ denotes the unique non-negative symmetric square root of T. By Γ being strongly continuous is meant that if $\{x_n\}_{n=0}^{\infty}$ is a sequence in H converging to $x \in H$ and $w \in H$, then

$$\lim_{n\to\infty} \Gamma(x_n)w = \Gamma(x)w.$$

Theorem 21.2. *Suppose* $w \in H, Q_0 = P$,

$$Q_{n+1} = Q_n^{1/2}\Gamma(Q_n^{1/2}w)Q_n^{1/2},\ n = 1, 2, \ldots.$$

Then

$$\{Q_n^{1/2}w\}_{n=1}^{\infty} \text{ converges to } z \in H$$

such that

$$Pz = z,\ \Gamma(z)z = z.$$

Proof. First note that Q_0 is symmetric and nonnegative. Using the fact that the range of Γ contains only symmetric and nonnegative members of $L(H,H)$, one has by induction that each of $\{Q_n\}_{n=1}^{\infty}$ is also symmetric and nonnegative. Moreover for each positive integer n, and each $x \in H$,

$$\langle Q_{n+1}x, x\rangle = \langle Q_n^{1/2}\Gamma(Q_n^{1/2}x)Q_n^{1/2}x, x\rangle \tag{21.6}$$
$$= \langle \Gamma(Q_n^{1/2}x)Q_n^{1/2}x, Q_x^{1/2}\rangle \le \langle Q_n^{1/2}x, Q_n^{1/2}x\rangle = \langle Q_n x, x\rangle, \tag{21.7}$$

so that $Q_{n+1} \le Q_n$. Hence $\{Q_n\}_{n=1}^{\infty}$ converges strongly on H to a symmetric nonnegative transformation Q and so also $\{Q_n^{1/2}\}_{n=1}^{\infty}$ converges strongly to $Q^{1/2}$. Denote by z the limit of $\{Q_n^{1/2}w\}_{n=1}^{\infty}$ and note that then

$$\{\Gamma(Q_n^{1/2}w)Q_n^{1/2}w\}_{n=1}^{\infty}$$

converges to $\Gamma(z)z$. Since for each positive integer $n, Q^{1/2}$ is the strong limit of a sequence of polynomials in Q_n, it follows by induction that $PQ^{1/2} = Q^{1/2}$. Hence $Pz = z$.

Since for each positive integer n and each $x \in H$,

$$\langle Q_{n+1}x, x\rangle = \langle \Gamma(Q_n^{1/2}w)Q^{1/2}x, Q^{1/2}x\rangle,$$

it follows that

$$\langle Qx, x\rangle = \langle Q^{1/2}x, Q^{1/2}x\rangle = \langle \Gamma(z)Q^{1/2}w, Q^{1/2}w\rangle$$

and hence

$$\langle (I - \Gamma(z))x, x\rangle = 0,\ x \in H$$

and so

$$(I - \Gamma(z))z = 0, \text{i.e.,} \Gamma(z)z = z.$$

This together with the already established fact that $Pz = z$ is what was to be shown. □

Further examples of a nonlinear projection methods are given in [57] (particularly Proposition 5) and in references contained therein.

Brown and O'Malley in [26] have generalized the above result. The next lemma and theorem give their result.

Lemma 21.3. *(From [26]) Let $Q \in B_1(H)$ and let α be a positive rational number other than 1. If $Q^\alpha = Q$, then $Q = Q^2$.*

Proof. Let $\alpha = r/s$; the presumed equality is equivalent to $Q^r = Q^s$. Assume that $r < s$ and that r is the minimal positive power of Q which reoccurs in the sequence $\{Q^n\}_{n=1}^{\infty}$. From the fact that powers of an operator descend in the quasi-order mentioned above, together with the limited anti-symmetry of this relation, it follows that $Q^t = Q^r$ for all integral t between r and s. From $Q^r = Q^{r+1}$, it follows that $Q^t = Q^r$ for all $t \geq r$. If r is odd, then

$$(Q^{(r+1)/2})^2 = Q^{r+1} = Q^{2r} = (Q^r)^2$$

By uniqueness of square roots, $Q^r = Q^{(r+1)/2}$ whence $r = (r+1)/2$ and $r = 1$. If r is even, then $(Q^{r/2})^2 = Q^r = (Q^r)^2$, whence $r = r/2$, which is impossible for positive r. Thus $r = 1$ and $Q = Q^2$. □

Theorem 21.4. *Let $w \in H$, let P be an orthogonal projection on H, and let $L : H \to B_1(H)$ be strongly continuous. Let α, β be positive rational numbers with $\alpha \in [1/2, \infty)$. Set $Q_0 = P$, and let*

$$Q_{n+1} = Q_n^\alpha L(Q_n^\beta w)Q_n^\alpha, \; n = 1, 2, \ldots.$$

Then $\{Q_n\}_{n=0}^{\infty}$ is a decreasing sequence of elements of $B_1(H)$ which converges to an element $Q \in B_1(H)$ such that (1) if $\alpha > 1/2$ then Q is idempotent and $z = Qw$ satisfies $L(z)z = z$ and $Pz = z$, and (2) if $\alpha = 1/2, \beta \geq 1/2$, then $z = Q^\beta w$ satisfies $L(z)z = z, Pz = z$.

Proof. (From [26].) Fix $\alpha \geq 1/2, \beta > 0$. Since $Q_0 = P \in B_1(H)$ and the range of L is in $B_1(H)$, it follows inductively that $Q_n \in B_1(H)$ for all n. Since $2\alpha \geq 1, Q_n^{2\alpha} \leq Q_n$; moreover,

$$\begin{aligned}\langle (Q_n^{2\alpha} - Q_{n+1})x, x\rangle &= \langle (Q_n^{2\alpha} - Q_n^\alpha L(Q_n^\beta w)Q_n^\alpha)x, x\rangle \\ &= \langle Q_n^\alpha (I - L(Q_n^\beta w))Q_n^\alpha x, x\rangle \\ &= \langle (I - L(Q_n^\beta w))Q_n^\beta w))Q_n^\alpha x, Q_x^\alpha\rangle.\end{aligned}$$

Thus, since $I - L(Q_n^\beta x) \geq 0$, if follows that $Q_{n+1} \leq Q_n^{2\alpha}$. Hence,

$$Q_{n+1} \leq Q_n^{2\alpha} \leq Q_n,\ n = 0, 1, 2, \ldots. \tag{21.8}$$

In particular, the sequence $\{Q_n\}_{n=1}^\infty$ is monotonically decreasing in the (operator) interval from 0 to I. Thus by [210] the sequence $\{Q_n^\alpha\}_{n=1}^\infty$ converges to Q^α and $\{Q_n^\beta\}_{n=1}^\infty$ converges to Q^β. Since L is continuous and operator multiplication is jointly continuous in the strong topology on $B_1(H)$, by uniqueness of limits

$$Q = Q^\alpha L Q^\beta(w) Q^\alpha.$$

Also from (21.8) and the closed graph of the relation $\leq$,

$$Q \leq Q^{2\alpha} \leq Q.$$

Thus, since $Q, Q^{2\alpha}$ commute, $Q = Q^{2\alpha}$. Moreover, since $P = Q_0$, $PQ_n = Q_n$, whence $PQ^\gamma = Q^\gamma$ for all positive rational γ.

(i) Suppose $\alpha > 0$. By (21.3) $Q = Q^2$, from which it follows that $Q = Q^\gamma$ for all positive rational γ, and in particular $Q = QL(Qw)Q$.

Let $z = Qw$, and fix $x \in H$.

$$\langle Qx, x\rangle = \langle QL(z)Qx, x\rangle = \langle L(z)Qx, Qx\rangle,$$

and since $Q^2 = Q$, it follows that

$$0 = \langle Qx, Qx\rangle - \langle L(z)Qx, Qx\rangle = \langle (I - L(z))Qx, Qx\rangle.$$

Therefore, since $I - L(z)$ and hence $(I - L(z))^{1/2}$ belong to $B_1(H)$, $Q = L(z)Q$. In particular, $z = Qw = L(z)Qw = L(z)z$.

(ii) Suppose $\alpha = 1/2, \beta \geq 1/2$. Let $z = Q^\beta w$; then $Q = Q^{1/2}L(z)Q^{1/2}$ from which

$$\langle Qx, x\rangle = \langle Q^{1/2}L(z)Q^{1/2}x, x\rangle = \langle L(z)Q^{1/2}x, Q^{1/2}x\rangle.$$

Since

$$\langle Qx, x\rangle = \langle Q^{1/2}, Q^{1/2}\rangle$$

it follows that

$$0 = \langle Q^{1/2}x - L(z)Q^{1/2}x, Q^{1/2}x\rangle = \langle (I - L(z))Q^{1/2}x, Q^{1/2}x\rangle.$$

Now as in (i), it follows that $Q^{1/2} = L(z)Q^{1/2}$. In particular,

$$z = Q^\beta w = Q^{1/2}Q^{\beta-1/2}w = L(z)Q^{1/2}Q^{\beta-1/2}w = L(z)Q^\beta w = L(z)z.$$

That $Pz = z$ in both cases is obvious from the fact that $PQ^\gamma = Q^\gamma$ for all positive rational γ. □

Further applications to differential equations are illustrated by the following simple case. Compare results of Chapter 3. Take A as a function from $L_2([0,1)])^2$ into $L(L_2([0,1])^2, L_2([0,1]))$ and take $D : H^{1,2}([0,1]) \to L_2([0,1])$ so that $Du = \binom{u}{u'}, u \in H^{1,2}([0,1])$. Make the assumption that

$$A(Du)A(Du)^* = I, \text{the identity on } L_2([0,1]),\ u \in H^{1,2}([0,1]),$$

a result that can be obtained by normalization granted that $A(Du)A(Du)^*$ is invertible. Define Γ so that

$$\Gamma(u) = u - A(Du)^* A(Du), u \in H^{1,2}([0,1]).$$

Take P to be the orthogonal projection of $L_2([0,1])$ onto $R(D)$. Then if $z \in H^{1,2}([0,1])$ and

$$Pz = z, \Gamma(z)z = z$$

hold, i.e., that the conclusion to Theorem 21.2 holds, it follows that

$$A(Du)Du = 0. \tag{21.9}$$

Equation (21.9) represents a substantial family of quasilinear differential equations.

The following problem from [146] is related to the above projection methods. Suppose H, K are two Hilbert spaces, P is an othogonal projection on H, $H, g \in K$ and B is a continuous linear transformation from H to K such that $BB^* = I$. Find y in H so that

$$By = g \text{ and } Py = y. \tag{21.10}$$

This is equivalent to finding $x \in H$ so that

$$BPx = g. \tag{21.11}$$

Make the definitions

$$L = I - B^*B, L_g x = Lx + B^*x, x \in H$$

and note that if $x \in H$, then $L_g x$ is the nearest element z to x so that $Bz = g$. Seek solutions x to (21.11) as

$$x = \lim_{n\to\infty} (PL_gP)^n z \text{ for some } z \in H.$$

First note that if $z \in H, g \in K$, then by induction

$$(PL_gP)^k z = (PLP)^k z + PB^*(I+(I-M)+\cdots+(I-M)^{k-1})g, k = 1, 2, \ldots \tag{21.12}$$

where

$$M = BPB^*$$

Note that M is a symmetric nonnegative linear transformation from K to K and $M \leq I$ so that the numerical range of M is a subset of $[0, 1]$. The next theorem gives a characterization of $\overline{R(BP)}$ and the one after that gives a characterization of $R(BP)$.

Theorem 21.5. *If* $g \in K$ *then* $g \in N(PB^*)^\perp$ *if and only if*

$$\lim_{k\to\infty} (I - M)^k g = 0.$$

Proof. Define $z = \lim_{k\to\infty} (I - M)^k g$. This limit exists since M is symmetric and $0 \leq I - M \leq I$. Now

$$(I - M)z = \lim_{k\to\infty} (I - M)^{k+1} g = z$$

so that $Mz = 0$ and hence $BPB^*z = 0$. Therefore

$$0 = \langle BPB^*z, z\rangle = \|PB^*z\|^2.$$

Hence $z \in N(PB^*)$. If in addition, $g \in N(PB^*)^\perp$, then

$$0 = \langle g, z\rangle = \langle g, \lim_{k\to\infty} (I - M)^{2k} g\rangle = \| \lim_{k\to\infty} (I - M)^k g\|^2 = \|z\|^2$$

and hence $z = 0$.

Now suppose that $z = 0$ and $w \in N(PB^*)$. Then

$$0 = \|z\|^2 = \langle \lim_{k\to\infty} (I - M)^k g, w\rangle = \langle g, \lim_{k\to\infty} (I - M)^k g, w\rangle = \langle g, w\rangle$$

since $(I - M)w = z$. Hence $\langle g, w\rangle = 0$ for all $w \in N(PB^*)$ and so $g \in N(PB^*)^\perp$. □

Theorem 21.6. *If* $g \in \overline{R(BP)}$ *then* $g \in R(BP)$ *if and only if*

$$\lim_{k\to\infty} PB^*(I + (I - M) + \cdots + (I - M)^{k-1})g$$

exists.

Proof. Suppose the limit in the theorem exists and call it z. Note that $Pz = z$. Then

$$\begin{aligned} Bz &= \lim_{k\to\infty} BPB^*(I + (I - M) + \cdots + (I - M)^{k-1})g \\ &= \lim_{k\to\infty} M(I + (I - M) + \cdots + (I - M)^{k-1})g \\ &= \lim_{k\to\infty} (g - (I - M)^k g) = g \end{aligned}$$

since $g \in \overline{R(BP)} = N(PB^*)^\perp$ and so by (21.5) $\lim_{k\to\infty}(I-M)^k g = 0$. Therefore $Bz = g$ and so $BPz = g$ since $Pz = z$. □

Theorem 21.7. *Suppose $g \in H, \lim_{k\to\infty}(I-M)^k g = 0$ and*

$$\lim_{k\to\infty} PB^*(I + (I-M) + \cdots + (I-M)^{k-1})g$$

exists. If $z \in H$, then $x = \lim_{k\to\infty}(PL_gP)^k z$ exists and satisfies $Px = x$, $Bx = g$, and hence $BPx = g$. Moreover, x is the nearest point w to z so that $Pw = w, Bw = g$.

Proof. Suppose $z \in H$. Define $r = \lim_{k\to\infty}(PLP)^k z$ and

$$y = PB^*(I + (I-M) + \cdots + (I-M)^{k-1})g.$$

Using (21.12),

$$x = \lim_{k\to\infty}(PL_gP)^k z = r + y.$$

But $Pr = r, Br = 0$ and, as in the proof of (21.6), $Py = y, By = g$. Therefore $Px = x, Bx = g$ and consequently $BPx = x$.

Suppose now that $w \neq x, Pw = w$. Then $BP(w-x) = g - g = 0$. Since $r = \lim_{k\to\infty}(PLP)^k z$, if follows that r is the nearest point of $R(P) \cap N(B)$ to z. Hence $\langle r - z, w - x\rangle = 0$ since $w - x \in R(P) \cap R(L)$. Also since for each positive integer k,

$$\begin{aligned}&\langle w - x, PB^*(I + (I-M) + \cdots + (I-M)^{k-1})g\rangle \\ &\quad = \langle BP(w-x), (I + (I-M) + \cdots + (I-M)^{k-1})g\rangle = 0,\end{aligned}$$

it follows that $\langle w - x, y\rangle = 0$. Hence x is the closest point w to z such that $Pw = w, Bw = g$. □

Apply the above development to a problem of functional differential equations with both advanced and retarded arguments. If $c \in R, f\ H = H^R$ then f_c denotes the member of H so that $f_c(t) = f(t+c), t \in R$. Suppose

$$\alpha, \beta > 0, g \in C^{(1)}(R), r, s \in C(R), r, s \text{ bounded.}$$

There is the problem of finding $f \in H$ so that

$$f' + rf_\alpha + sf_{-\beta} = g. \tag{21.13}$$

This is a functional differential equation with both advanced and retarded arguments [53, 77]. Define $A : L_2(R)^2 \to L_2(R)$ by

$$A\binom{f}{g} = g + rf_\alpha + sf_{-\beta}, f, g \in L_2(R)^2. \tag{21.14}$$

Lemma 21.8. *Suppose A satisfies (21.14). Then*

$$A^*z = \binom{(rz)_{-\alpha}+(sz)_\beta}{z}, z \in L_2(R).$$

Moreover, AA^* has a bounded inverse defined on all of $L_2(R)$.

Proof. For $\binom{f}{g} \in L_2(R)^2, z \in L_2(R)$

$$\begin{aligned}\langle A\tbinom{f}{g}, z\rangle_{L_2(R)} &= \int_{-\infty}^{\infty} (rf_\alpha + sf_{-\beta} + g)z \\ &= \int_{-\infty}^{\infty} (f(rz)_{-\alpha} + f(sz)_\beta + gz) = \langle \tbinom{f}{g}, \tbinom{((rz)_{-\alpha}+(sz)_\beta}{z})\rangle_{L_2(R)}.\end{aligned}$$

The first conclusion then follows. To get the second, compute

$$\begin{aligned}AA^*z &= z + r[(rz)_{-\alpha} + (sz)_\beta]_\alpha + s[(rz)_{-\alpha} + (sz)_\beta]_{-\beta} \\ &= (1 + r^2 + s^2)z + r(sz)_{\alpha+\beta} + s(rz)_{-\alpha-\beta} = (I + CC^*)z\end{aligned}$$

where

$$C\tbinom{f}{g} = rf_\alpha + sf_{-\beta},\ \tbinom{f}{g} \in L_2(R)^2.$$

It is then clear that the second conclusion holds. □

Define $B = (AA^*)^{1/2}A$. Then B satisfies the hypothesis of the previous three theorems.

Lemma 21.9. *The orthogonal projection Q of $L_2(R)^2$ onto*

$$\{\tbinom{u}{u'},\ u \in H^{1,2}(R)\} \text{ is given by } Q\tbinom{f}{g} = \tbinom{u}{u'}$$

where

$$\begin{aligned}u(t) = (e^t/2)&\int_t^\infty e^{-s}(f(s) - g(s))\,ds \\ &+ (e^{-t}/2)\int_{-\infty}^t e^s(f(s) + g(s))\,ds, t \in R.\end{aligned}$$

Proof. Note that Q is idempotent, symmetric and fixed on all points of $\{\binom{u}{u'} : u \in H_{1,2}(R)\}$ and has range in this set. This is enough to show that Q is the required orthogonal projection. □

The formula in Lemma 21.9 came from a calculation like that of the problem in Section 5.1 of Chapter 5. On this infinite interval one has the requirement that various functions are in $L_2(R)$ but there are no boundary conditions.

With A as in Lemma 21.8 and P as in Lemma 21.9, form B as above and take $M = BPB^*$. If the conditions of Theorem 21.7 are satisfied one is assured of existence of a solution to (21.13). Linear functional differential equations in a region $\Omega \subset R^m$ for $m > 1$ may be cast similarly. As an alternative to these projection methods, one can use the continuous steepest descent propositions of Chapters 3 and 4 and numerical techniques similar to those of Chapter 8. We do not have concrete results of functional differential equations to offer as of this writing but it is suspected that there are possibilities along the lines indicated. For references on functional differential equations in addition to [53,77] and references [12,207,224]. In this last reference there are refinements to some of the propositions of this chapter.

Chapter 22
An Analytic Iteration Method

This chapter deals with an iteration scheme for partial differential equations which, at least for this writer, provided another predecessor theory to the main topic of this monograph. Investigations leading to the main material of this monograph started after a failed attempt to make numerical the material of the present chapter. The scheme deals with spaces of analytic functions, almost certainly not the best kind of spaces for partial differential equations. To deal with these iterations, some notation concerning higher derivatives is needed.

Suppose that each of m and n is a positive integer and u is a real valued $C^{(n)}$ function on an open subset of R^m. For $k \leq n$ and x in the domain of u, $u^{(k)}(x)$ denotes the derivative of order k of u at x - it is a symmetric $k-linear$ function on R^m (cf [170]).

Denote by $M(m,n)$ the vector space of all real-valued $n-linear$ functions on R^m and for $v \in M(m,n)$ take

$$\|v\| = (\sum_{p_1=1}^{m} \cdots \sum_{p_n=1}^{m} (v(e_{p_1}, \ldots, e_{p_n})))^{1/2} \tag{22.1}$$

where $e_1, \ldots, e_m$ is an orthonormal basis of R^m. As Weyl points out in [226], p 139, the expression in (22.1) does not depend on particular choice of orthonormal basis. Note that the norm in (22.1) carries with it an inner product.

Denote by $S(m,n)$ the subspace of $M(m,n)$ which consists of all symmetric members of $M(m,n)$ and denote by $P_{m,n}$ the orthogonal projection of $M(m,n)$ onto $S(m,n)$. For $y \in R^m, v \in S(m,n)$, vy^n denotes $v(y_1, \ldots, y_n)$ where $y_j = y,\ i = 1, \ldots, n$.

Suppose $r > 0$ and u is a $C^{(n)}$ function whose domain includes $B_r(0)$. Notice the Taylor formula:

$$u(x) = \sum_{q=0}^{n-1} u^q(0)x^q + \int_0^1 ((1-s)^{n-1}/(n-1)!)u^{(n)}(sx)x^n\, ds. \tag{22.2}$$

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For $A, w \in S(m,n)$, Aw denotes the inner product of A with w taken with respect to (22.1).

Now suppose that k is a positive integer, $k < n$, f is a continuous function from

$$R^m \times R \times S(1,n) \times \cdots \times S(k,n) \to R$$

and A is a member of $S(m,n)$ with $\|A\| = 1$. Given $r > 0$ one has the problem of finding $u \in C^{(n)}$ so that

$$Au^{(n)}(x) = f(x, u(x), u'(x), \ldots, u^{(k)}(x)),\ \|x\| \le r. \tag{22.3}$$

Abbreviate the rhs of (22.3) by $f_u(x)$.

To introduce our iteration method, note that if $v \in S(m,n), g \in R$ then

$$v - (Av - g)A$$

is the nearest element w of $S(m,n)$ to v so that $Aw = g$. This observation together with (22.2) leads us to define

$$T : C^{(n)}(B_r(0)) \to C(B_r(0))$$

by

$$(Tv)(x) = \sum_{q=0}^{n-1} v^q(0)x^q + \int_0^1 ((1-s)^{n-1}/(n-1)!) \tag{22.4}$$

$$(v^{(n)}(sx) - (Av^{(n)}(sx) - f_v(sx))A)x^n\ ds,\ \|x\| \le r,\ v \in C^{(n)}(B_r(0)). \tag{22.5}$$

Consider the possible convergence of

$$\{(T^j v)(x)\}_{j=1}^{\infty} \tag{22.6}$$

at least for $\|x\| \le \rho$ with $0 < \rho \le r$. This convergence is a subject of a series of papers [141–144] and [177–181]. Some results from these papers are indicated in what follows.

For $r > 0$ denote by α_r the collection of all real-valued functions v so that

$$v(x) = \sum_{q=0}^{\infty} (1/q!) v^{(q)} x^q, \sum_{q=0}^{\infty} (1/q!) \|v^{(q)}\| x^q < \infty,\ \|x\| \le r. \tag{22.7}$$

Theorem 22.1. *If $r > 0, u \in C^{(n)}(B_r(0))$, then $Tu = u$ if and only if* (22.3) *holds.*

Theorem 22.2. *Suppose $r > 0$ and h is a real-valued polynomial on R^m, $A \in S(m,n)$ with $\|A\| = 1$ and*

$$(Tv)(x) = \sum_{q=0}^{n-1} v^q(0)x^q + \int_0^1 ((1-s)^{n-1}/(n-1)! \tag{22.8}$$

$$(v^{(n)}(sx) - (Av^{(n)}(sx) - h(sx))A)x^n \; ds, \|x\| \le r, v \in \alpha_r. \tag{22.9}$$

Then $\{T^j v\}_{j=0}^{\infty}$ *converges uniformly on* $B_r(0)$ *to* $u \in \alpha_r$ *such that*

$$Au^{(n)}(x) = h(x), \; \|x\| \le r.$$

The next two theorems require a lemma from [142]. In order to state the lemma, some additional notation is needed. There are several kinds of tensor products which will be used. Suppose that each of n, k is a positive integer, $n \le k$, i is a nonnegative integer, $i \le n$. For $A \in S(m,n), D \in S(m,k)$ define $A \otimes_i D$ to be the member $w \in S(m, n+k-2i)$ so that

$$w(y_1, \ldots, y_{n+k-2i}) = \langle A(y_1, \ldots, y_{n-i}), D(y_{n-i+1}, \ldots, y_{n+k-2i} \rangle,$$
$$y_1, \ldots, y_{n+k-2i} \in R^m,$$

where the above inner product $\langle \; , \; \rangle$ is taken in $S(m,i)$. The case $i = 0$ describes the usual tensor product of A and D; the case $i = n$ describes what will be called the inner product of A and D and in this case $A \otimes_n D$ is denoted simply as $AD \in S(m, k-n)$ and is called AD the inner product of A with D. If $k = n$ the this agrees with our previous convention. The symmetric product $A \vee D$ is defined as $P_{m,n}(A \otimes D)$.

The following lemma is crucial to proving convergence of our iteration in nonlinear cases. It took about seven years to find; an argument is found in [142].

Lemma 22.3. *If* $A, C \in S(m,n), B, D \in S(m,k)$ *and* $n \le k$, *then*

$$\binom{n+k}{n} \langle A \vee B, C \vee D \rangle = \sum_{i=0}^{n} \binom{n}{i} \binom{k}{i} \langle A \otimes_i D, C \otimes_i B \rangle. \tag{22.10}$$

Observe that the lemma has the easy consequence

$$\|A \vee B\|^2 \ge \binom{n+k}{n}^{-1} \|A\|^2 \|B\|^2. \tag{22.11}$$

This inequality is crucial to the following (essentially from [143, 144]):

Theorem 22.4. *Suppose that* $r > 0, v \in \alpha_r$ *and* f *in* (22.3) *is real-analytic at*

$$(0, v(0), v'(0), \ldots, v^{(k)}(0)) \in R^m \times R \times S(1,n) \times \cdots \times S(k,n).$$

If $k \le n/2$ there is $\rho \in (0, r]$ so that $\{T^j v\}_{j=0}^{\infty}$ converges uniformly on $B_\rho(0)$ to $u \in \alpha_\rho$ such that

$$Au^{(n)}(x) = f_u(x),\ \|x\| \le \rho.$$

In [178] Pate generalizes the above in the direction of weakening the requirement $k \le n/2$. The key is an analysis of higher order terms of

$$\binom{n+k}{n} \|A \vee B\|^2 = \sum_{i=0}^{n} \binom{n}{i} \binom{k}{i} \|A \otimes_i B\|^2$$

which is just (22.10) with $C = A \in S(m,n), D = B \in S(m,k)$. The main fact in this analysis is the result from [177] that

$$\binom{n+k}{n} \|A \vee B\|^2 \ge \sum_{i=0}^{\min(n/2,k)} \binom{n}{i} \binom{k}{i} \|A \otimes B\|^2 \mu_q(A)$$

where for $0 \le q \le \min(n/2, k)$, $\mu_q(A)$ is defined to be $\lambda_q(A)/\|A\|^2$ and $\lambda_q(A)$ is defined as follows: For q in this range and A a non zero member of $S(m,n)$ define

$$A_q : S(m,q) \to S(m, n-q)$$

by $A_q u = Au$, the above defined 'inner product' of A and u. Then denote $A_q^t : S(m, n-q) \to S(m,n)$ the corresponding adjoint transformation. Finally, define $T_q : S(m,n) \to S(m,n)$ by $T_q u = A_q^t(A_q u), u \in S(m,n)$. Then $\lambda_q(A)$ is the minimum eigenvalue of T_q.

In [178], the condition $k \le n/2$ of (22.4) is weakened to state $k \le (n+j)/2$ where j is the largest integer p such that $\lambda_p(A) \ne 0$. This is a result of some deep and difficult mathematics. The reader is encouraged to see [177–181] for details.

A result from [141] has to do with the following: Suppose that a, b, c are three pair-wise linearly independent elements of R^2 and A, B, C are the elements dual to a, b, c respectively, i.e.,

$$Ax = \langle x, a \rangle_{R^2},$$

and similarly for the pairs (B, b),(C, c). Let

$$Q = A \vee B \vee C \in S(2,3).$$

Consider the problem of finding $u : R^2 \to R$ such that

$$Qu'''(x,y) = 0,\ (x,y) \in R^2. \tag{22.12}$$

Theorem 22.5. *If* L_A, L_B, L_C *are the three lines through* $(0, 0, 0)$ *which are orthogonal to* a, c, b *respectively and* f *is an analytic function on* R^3*, there is a unique analytic function* u *so that* u *agrees with* f *on each of* L_A, L_B, L_C *and* (22.12) *holds.*

Aside from the algebraic work of Pate cited above, almost nothing has been continued from the work in [141, 143, 144]. It is suspected that there is a lot more to be found in this area.

Attempts to extend by continuity work in [141] beyond the class of analytic functions led to work on quasi-analyticity (see [162] and earlier references contained therein). It still seems possible for such extensions to be made.

Chapter 23
Steepest Descent for Conservation Equations

Many systems of conservation equations may be written in the form

$$u_1 = \nabla \cdot F(u, \nabla(u)) \tag{23.1}$$

where for some positive integers n, k and $T > 0$ and some region

$$\Omega \subset R^n, u : [0, T] \times \Omega \to R^k.$$

Often, however, a more complicated form is encountered:

$$(Q(u))_1 = \nabla \cdot F(u, \nabla(u)),\ S(u) = 0 \tag{23.2}$$

where here for some positive integer q,

$$\begin{aligned} &u : [0, T] \times \Omega \to R^{k+q}, \\ &Q : R^{k+q} \to R^k, S : R^{k+q} \to R^q, \\ &F : R^{k+q} \times R^{n(k+q)} \to R^{nk}. \end{aligned}$$

The condition $S(u) = 0$ in (23.2) is a relationship between the components of the unknowns u. It is often called an equation of state. In $Q(u)$ unknowns may be multiplied as in momentum equations. Sometimes (23.2) can be changed into (23.1) by using the condition $S(u) = 0$ to eliminate q of the unknowns and by using some change of variables to convert the term $(Q(u))_1$ into the form u_1, but it often seems better to treat the system (23.2) numerically just as it is written.

Consider homogeneous boundary conditions on $\partial\Omega$ as well as initial conditions. A strategy is described for a time-stepping procedure. Take w to be a time-slice of a solution at time t_0. Seek an estimate v at time $t_0 + \delta$ for some time step δ. Seek v as a minimum to ϕ where

$$\phi(v) = [\|Q(v) - Q(w) - \delta F((w + v)/2, \nabla((v + w)/2))\|^2 + \|S((v + w)/2)\|^2$$

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for all v $H^{2,2}(\Omega, R^n)$ satifying the homogeneous boundary conditions. If v is found so that $\phi(v) = 0$, then it may be a reasonable approximation of a solution at $t_0 + \delta$. Assuming that F and Q are such that ϕ is a $C^{(1)}$ function with locally lipschitzian derivative, theory in various preceeding chapters may be applied in order to arrive at a zero (or at least a minimum) of ϕ. In particular consider continuous steepest descent

$$z(0) = w, z'(t) = -(\nabla\phi)(z(t)),\ t \geq 0 \tag{23.3}$$

where the descent started at w, the time slice estimating the solution at t_0. If δ is not too large, then w should be a good place to start an iteration. For numerical computations there is interest in tracking (23.3) numerically with a finite number of steps. This procedure was tested on Burgers' Equation

$$u_1 + uu_2 = \nu\Delta u$$

with periodic boundary conditions. The above development is taken from [156]. A more serious application is reported in [158] for a magnetohydrodynamical system consisting of eight equations (essentially a combination of Maxwell's equations and Navier-Stokes equations) together with an equation of state. These equations were taken from [211] and the computations was carried out in three space dimensions. The code has never been properly evaluated but it seemed to work.

Chapter 24
Code for an Ordinary Differential Equation

Figure 24.1 gives a MatLab code for obtaining numerical solutions to the problem of finding $u : [0,1] \to R$ so that

$$u' - u - 0 \tag{24.1}$$

on the interval $[0,1]$. Much more complicated problems follow the same logic in that a conventional gradient is first calculated and then a Sobolev gradient is obtained from this conventional gradient in a way indicated by the theory of the present work.

We go through items in the code. The integer n is the number of pieces into which the interval $[0,1]$ is broken for a discretization of the problem. The term er specifies an error tolerance below which the main iteration is terminated. The next five lines essentially reserve space for needed arrays. The code is much faster using sparse arrays and it permits n to be at least 10^6 (without sparse arrays, the inverse of q would have 10^{12} entries, all positive). The loop to follow sets up needed sparse matrices, $d1$ for approximating first order differences and $d0$ for an approximation to the identity function on the grid, The second loop specifies an initial estimate u on the grid. The array q is the appropriate 'D^tD' of Chapter 10. Its inverse is the imbedding transformation M associated with the pair of spaces H, whose points are those of R^{n+1}, with norm

$$\|u\|^2 = \sum_{k=0}^{n} u(k)^2,\ u \in R^{n+1},$$

and H' whose points are also those of R^{n+1} but with norm

$$\|u\|_{H'} = \sum_{k=1}^{n}((\frac{1}{n}(u(k) - u(k-1)))^2 + (\frac{1}{2}(u(k) + u(k-1)))^2.$$

The term f is an array so that if $u \in H$ and

$$fu = 0$$

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```
format long e
n = 1000;
er = 1.e-12;
u = ones(n+1,1);
i0 = zeros(2*n,1);
j0 = zeros(2*n,1);
s0 = zeros(2*n,1);
s1 = zeros(2*n,1);
for k=1:1:n
j0(k)=k;
j0(k+n)=k+1;
i0(k)=k;
i0(k+n)=k;
s0(k)=.5;
s0(k+n)=.5;
s1(k)=-n;
s1(k+n)=n;
end
d1 = sparse(i0,j0,s1);
d0 = sparse(i0,j0,s0);
for k=1:1:n+1
x = (k-1)/n;
u(k) = 1/(x+1);
end
q = d0'*d0 + d1'*d1;
f = d1 - d0;
xx = 10;
mc = 0;
while xx > er
g = q\(f'*f*u);
step = (f*u)'*(f*g)/((f*g)'*(f*g));
u = u - step*g;
xx = g'*g;
mc = mc + 1;
end
mc,step,xx
plot(u)
```

Fig. 24.1 MatLab Code

then u is a solution to the finite difference problem, for n divisions of $[0, 1]$ of (24.1). The term xx holds the norm of residuals at various steps of the iteration. It is initialized to be large. The term mc denotes a counter which keeps account of the step number as an iteration proceeds. The term g, at each step of the iteration, is essentially the inverse of q times the ordinary gradient. Thus g represents a Sobolev gradient. The term *step* computes the optimal size for a step at given iteration. Next is xx, measuring the square of the norm of the Sobolev gradient, a small value indicating that one is close to convergence.

The code in Figure 24.1 is for the case of no boundary conditions. By varying the initial estimate u one gets a variety of solutions. One may check that the limiting value of u is essentially the nearest solution in the H' norm to the initial estimate as it is in the continuous case.

To introduce initial conditions, for example, the code may be modified in a rather straigtforward way (see Chapter 8). One way to *NOT* get a proper Sobolev gradient for the related initial value problem is to simply zero out the Sobolev gradient calculated for no boundary conditions (the present case). Instead developments in Chapter 8 should be followed.

Most of the codes written which implement Sobolev gradients are written in FORTRAN or C. Using MatLab, the logic is essentially identical. The main benefit of MatLab lies in its provision of good linear solvers. Here the linear solver is used in the line in which g is obtained from f and u by means of solving a linear system with matrix q and right hand side the ordinary gradient.

Chapter 25
Geometric Curve Modeling with Sobolev Gradients

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The Sobolev gradient method is a powerful tool for geometric modeling. We treat the problem of constructing fair curves by minimizing a fairness measure subject to geometric constraints. The measure might include curve length, curvature, torsion, and/or variation of curvature. The constraints may include specified values, tangent vectors, and/or curvature vectors. We may also require periodicity in the case of closed curves, or nonlinear inequalities representing shape-preservation criteria. The curve is represented by discrete vertices and divided difference approximations to derivatives with respect to arc length. A Sobolev gradient method is then particularly effective for minimizing the functional.

25.1 Introduction

Our first application of the Sobolev gradient method to a geometric modeling problem involved the construction of a surface with minimal surface area and constrained to pass through a space curve in Chapter 16. The analogous curve-fitting problem is the construction of the minimum-length curve that passes through a pair of points. The problem is trivial in that the solution is just the line segment defined by the endpoints, but as a numerical optimization problem, it is not uninteresting. We will show that standard methods are doomed to failure, while a generalization of the Sobolev gradient method produces the solution in a single iteration. The latter observation was the starting point for our work in [190].

We restrict attention here to the simple minimum-length curve problem. While this problem is sufficient to demonstrate the key ideas, more complex applications involve a number of algorithmic details that can strongly affect the efficiency of the method, and we refer the reader to the literature for more extensive discussion. In [192] we treated the problem of interpolation with nonlinear splines, and in [193] we discussed the more general problem of constructing parametric space curves that minimize variation of curvature and take on pre-specified values, tangent vectors, and curvature vectors. The

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problem of constructing elastic curves constrained to lie in a regular surface is treated in [194], and [110] is addressed to the construction of periodic closed geodesics in a regular surface. Finally, in [195] we extended the work of [193] to handle inequalities representing shape-preservation criteria.

In the following section we discuss the minimum curve-length problem in the function space setting. Section 3 is addressed to the discretized problem, and test results are presented in Section 4.

25.2 Minimum Curve-Length

We reiterate here the discussion at the beginning of Chapter 16. The distinction between planar curves and space curves is not important. For $n = 2$ or $n = 3$ the set of C^2 regular parametric curves in $\mathbf{R}^n$ is

$$\mathcal{C} = \{f \in \left(C^2[0,1]\right)^n : f'(t) \neq 0 \quad \forall t \in [0,1]\}.$$

We also need a space of perturbations which preserve the endpoint values of elements of $\mathcal{C}$:

$$\mathcal{C}_o = \{h \in \left(C^2[0,1]\right)^n : h(0) = h(1) = 0\}.$$

The curve length functional is $\phi : \mathcal{C} \to \mathbf{R}$ defined by

$$\phi(f) = \int_0^1 \|f'(t)\|\, dt = \int_0^1 s'(t)\, dt,$$

where s is arc length associated with f. We may think of the curve as a trajectory of a moving particle, in which case t represents time, $f'(t)$ is a velocity vector tangent to the curve at $f(t)$, $s(t)$ is the arc length traversed between times 0 and t, and $s'(t)$ is speed.

The set of regular curves $\mathcal{C}$ has no zero element, and is therefore not a linear space. Rather it is an infinite-dimensional manifold. In order to define a metric on $\mathcal{C}$, we must define an inner product on the tangent space at each point $f \in \mathcal{C}$. Using the L_2 inner product, the L_2 gradient $\nabla\phi(f)$ is defined by $\phi'(f)h = \langle \nabla\phi(f), h\rangle_{(L_2[0,1])^n} \quad \forall h \in \mathcal{C}_o$, where the Fréchet derivative of ϕ at f in the direction h is

$$\phi'(f)h = \int_0^1 \frac{\langle f', h'\rangle}{\|f'\|}\, dt, \tag{25.1}$$

and

$$\nabla\phi(f) = -\left(\frac{f'}{\|f'\|}\right)' = -\|f'\|\kappa N \tag{25.2}$$

for curvature vector κN, by (16.2) and the equations that follow (16.1). Thus, as one would expect, a critical point of ϕ has zero curvature. The minimization problem does not have a unique solution, however, since the line segment does not have a unique parameterization. Consider a steepest descent method for minimizing ϕ. The curves evolve in the negative gradient direction which, using the L_2 gradient, is toward the center of curvature at each point on the curve. This seems to make sense. However, the parameter-dependent scale factor $\|f'\|$ is not appropriate and, more importantly, the L_2 gradient lacks smoothness. Each descent step reduces the number of continuous derivatives by two.

In order to demonstrate the relationship of our formulation with the standard Sobolev gradient setup, define a first-order differential operator D_f by

$$D_f h \equiv \frac{h'}{\sqrt{s'}} \quad \forall h \in \mathcal{C}_o.$$

Then the adjoint operator D_f^* is defined by

$$\begin{aligned}\langle h, D_f^* k\rangle_{(L_2[0,1])^n} = \langle D_f h, k\rangle_{(L_2[0,1])^n} &= \int_0^1 \frac{\langle h', k\rangle}{\sqrt{s'}}\, dt \\ = \int_0^1 \left\langle h, -\left(\frac{k}{\sqrt{s'}}\right)'\right\rangle dt &= \left\langle h, -\left(\frac{k}{\sqrt{s'}}\right)'\right\rangle_{(L_2[0,1])^n}\end{aligned}$$

for all $k, h \in \mathcal{C}_o$ so that

$$D_f^* k = -\left(\frac{k}{\sqrt{s'}}\right)',$$

and the negative f Laplacian $L_f \equiv D_f^* D_f$ is given by

$$L_f(h) = D_f^* D_f h = -\left(\frac{h'}{s'}\right)'. \tag{25.3}$$

The Fréchet derivative $\phi'(f)$ is a bounded linear functional on $\mathcal{C}_o$ with the f inner product (16.2) as well as the L_2 inner product. By the Riesz Representation Theorem it is therefore uniquely represented by the f gradient $g \equiv \nabla_f \phi(f) \in \mathcal{C}_o$. Thus, for all $h \in \mathcal{C}_o$,

$$\begin{aligned}\phi'(f)h = \langle \nabla\phi(f), h\rangle_{(L_2[0,1])^n} &= \langle g, h\rangle_f \\ = \int_0^1 \frac{\langle g', h'\rangle}{s'}\, dt &= \langle D_f g, D_f h\rangle_{(L_2[0,1])^n} \\ = \langle D_f^* D_f g, h\rangle_{(L_2[0,1])^n},&\end{aligned}$$

so that

$$\nabla\phi(f) = D_f^* D_f g = L_f(g). \tag{25.4}$$

Denote by P_o the orthogonal projection onto the space of parametric curves h that satisfy homogeneous end conditions $h(0) = h(1) = 0$. Then the restriction of $P_o L_f$ to $\mathcal{C}_o$ is invertible, and its inverse serves as a smoothing operator for the gradient:

$$\nabla_f \phi(f) = \left(P_o L_{f|\mathcal{C}_o}\right)^{-1} \nabla\phi(f). \tag{25.5}$$

Since the Sobolev gradient g is based on a metric that varies with f, a descent method using g is, like a quasi-Newton method, a variable metric method.

For more general problems the trick to choosing the right inner product on the tangent space at f is to retain independence from the parameterization by using derivatives with respect to arc length along f, and make the highest order of differentiation agree with that of the functional whose critical points are sought. When higher order derivatives are involved there remains some flexibility in choosing their relative weights. The weights used in the inner product need not agree with those appearing in the functional. The weights in the functional define the properties of the solution curve, while those in the inner product affect computational efficiency. Placing more weight on the low-order derivatives improves the condition number of the smoothing operator but may make it less effective, requiring more descent steps for convergence. Optimal weights are problem-dependent.

Returning to the curve-length problem, let $u = f - g$, corresponding to a single step of steepest descent with step-length 1. The following trivial but surprising theorem shows that u is the solution to the minimization problem.

Theorem 25.1. *Let $u = f - g$ for $g = \nabla_f \phi(f)$. Then $\nabla\phi(u) = 0$.*

Proof. By (2), (3), and (4), $L_f(f)$ and $L_f(g)$ are both equal to $\nabla\phi(f)$, so that

$$-L_f(u) = \left(\frac{u'}{s'}\right)' = \frac{s'u'' - s''u'}{(s')^2} = 0,$$

implying that u'' and u' have the same direction, and u therefore has zero curvature. □

Equation (16.5) characterizes the solution u more precisely as a line segment parameterized by the arc length along the initial curve f.

An alternative inner product is defined by $\langle g, h\rangle_{H(f)} = \langle H(f)g, h\rangle_{(L_2[0,1])^n}$, when the Hessian $H(f)$ is positive definite on $\mathcal{C}_o$. In general the curve Laplacian L_f is a preconditioner whose effectiveness depends on how close it is to $H(f)$. In order to obtain an expression for the Hessian, we compute the second derivative at f in the directions $h, k \in \mathcal{C}_o$. Using (1),

$$\begin{aligned}
\phi''(f)hk &= \int_0^1 \langle k, H(f)h\rangle \, dt = \lim_{\alpha\to 0} \frac{1}{\alpha}\left[\phi'(f+\alpha k)h - \phi'(f)h\right] \\
&= \lim_{\alpha\to 0} \frac{1}{\alpha}\int_0^1 \frac{\langle f'+\alpha k', h'\rangle}{\|f'+\alpha k'\|} - \frac{\langle f', h'\rangle}{\|f'\|}\, dt \\
&= \lim_{\alpha\to 0} \frac{1}{\alpha}\int_0^1 \frac{\|f'\|\langle f'+\alpha k', h'\rangle - \|f'+\alpha k'\|\langle f', h'\rangle}{\|f'+\alpha k'\|\|f'\|}\, dt \\
&= \int_0^1 \frac{\langle k', h'\rangle}{\|f'\|} + \lim_{\alpha\to 0}\frac{1}{\alpha}\int_0^1 \frac{\langle f', h'\rangle\left(\|f'\| - \|f'+\alpha k'\|\right)}{\|f'+\alpha k'\|\|f'\|}\, dt \\
&= \int_0^1 \left[\frac{\langle k', h'\rangle}{\|f'\|} - \frac{\langle f', h'\rangle\langle f', k'\rangle}{\|f'\|^3}\right] dt \\
&= \int_0^1 \left[\langle k', h'\rangle - \langle \Delta\mathbf{f}, h'\rangle\langle \Delta\mathbf{f}, k'\rangle\right]/s'\, dt \\
&= \int_0^1 \langle k', h' - \langle \Delta\mathbf{f}, h'\rangle \Delta\mathbf{f}\rangle /s'\, dt \\
&= \int_0^1 \left\langle k', \left(I - \Delta\mathbf{f}\Delta\mathbf{f}^T\right)h'\right\rangle /s'\, dt \\
&= \int_0^1 \left\langle \frac{k'}{\sqrt{s'}}, \left(I - \Delta\mathbf{f}\Delta\mathbf{f}^T\right)\frac{h'}{\sqrt{s'}}\right\rangle dt \\
&= \int_0^1 \left\langle D_f k, \left(I - \Delta\mathbf{f}\Delta\mathbf{f}^T\right)D_f h\right\rangle dt \\
&= \int_0^1 \left\langle k, D_f^*\left(I - \Delta\mathbf{f}\Delta\mathbf{f}^T\right)D_f h\right\rangle dt,
\end{aligned}$$

where $\Delta\mathbf{f}(t) \equiv f'(t)/\|f'(t)\|$ is the unit tangent vector at $f(t)$. The Hessian is thus

$$H(f) = D_f^*\left(I - \Delta\mathbf{f}\Delta\mathbf{f}^T\right)D_f.$$

This operator differs from L_f only in the term $I-\Delta\mathbf{f}\Delta\mathbf{f}^T$ which projects onto the orthogonal complement of $\Delta\mathbf{f}$. If we replace L_f by $H(f)$ in a steepest descent method, we have a damped Newton iteration. The following theorem shows that such a method is doomed to failure: the linear systems become increasingly ill-conditioned as the iteration proceeds.

Theorem 25.2. *The Hessian of ϕ is singular at a critical point.*

Proof. A critical point f is a parameterized line segment with constant unit tangent vector $\Delta\mathbf{f}$. Let $k(t) = \sin(2\pi t)\Delta\mathbf{f}$. Then k is a nonzero element of $\mathcal{C}_o$, but $D_f k$ has direction $\Delta\mathbf{f}$ and hence lies in the null space of $I - \Delta\mathbf{f}\Delta\mathbf{f}^T$, so that k is in the null space of $H(f)$. □

The singular Hessian is unusual. More typical behavior occurs in the problem of minimization of surface area. The Hessian of that functional, rather than being singular at a critical point, is positive definite only in the vicinity of a local minimum. In treating that problem we found it advantageous to switch from a Sobolev gradient descent method to a Newton iteration when the approximate solution was accurate enough for the Hessian to be positive definite. In some cases, however, we encountered numerical difficulties associated with nonuniqueness of the parameterization of critical points. That problem was solved by using an alternative to the surface area functional. The analogous alternative for curve length is the following parameter-dependent functional:

$$\psi(f) = \frac{1}{2}\int_0^1 \|f'(t)\|^2\,dt.$$

The negative L_2 gradient, $-\nabla\psi(f) = f''$, is the acceleration vector, and with the endpoint constraints, ψ is therefore uniquely minimized by the constant-speed line segment $f(t) = f(0) + t[f(1) - f(0)]$. Using $Dh = h'$, the negative Laplacian and the Hessian of ψ are both defined by $D^*Dh = -h''$ so that the Sobolev gradient descent method with step-length 1 is a Newton iteration, and converges in one iteration. Since ψ is quadratic, this is no surprise. We use a discretization of ψ as a regularization term for constructing minimum variation curves ([193]). It not only serves as a tension factor, preventing extraneous loops, but also helps to maintain uniformly distributed vertices.

25.3 Discrete Minimum-Length Curves

We now consider the discretized minimum curve-length problem. In order to keep the notation simple, we retain some of the same symbols used in the function space setting. Although not significant for the simple problem treated here, a key idea is to represent a curve by an ordered sequence of discrete vertices. Then segment arc lengths are distances between vertices, and derivatives with respect to arc length are approximated by simple divided differences. The total curvature, for example, is a sum of squared second differences scaled by segment lengths. With a finite element formulation, on the other hand, the total curvature would be represented by a complicated formula involving a parameter t, and would require a high-order quadrature method to control the discretization error. To reiterate, there is no need to explicitly discretize the domain $[0, 1]$. We implicitly assume a constant time interval Δt associated with each segment so that constant speed corresponds to uniformly distributed vertices.

A discrete curve $\mathbf{f}$ is a sequence of $m + 1$ vertices $\mathbf{f}_i \in \mathbf{R}^n, i = 0, \ldots, m$, $m \geq 2$, where adjacent vertices are distinct, and $\mathbf{f}_0$ and $\mathbf{f}_m$ are distinct fixed endpoints. One might think of $\mathbf{f}$ as the polygonal curve (piecewise linear interpolant) associated with the vertices, but it should not be identified with a C^0 parametric spline curve. Only the endpoints are control points. In general, there are many more vertices than control points, and there are discretized derivative vectors along with the vertices. The sequence of vertices should be thought of as a discrete representation of a C^2 parametric curve.

Denote segment lengths by Δs_i, unit tangent vectors by $\Delta \mathbf{f}_i$, and vertex normal curvature vectors by $\Delta^2 \mathbf{f}_i$:

$$\begin{aligned} \Delta s_i &= \|\mathbf{f}_i - \mathbf{f}_{i-1}\| \quad (i = 1, \ldots, m), \\ \Delta \mathbf{f}_i &= \frac{\mathbf{f}_i - \mathbf{f}_{i-1}}{\Delta s_i} \quad (i = 1, \ldots, m), \\ \Delta^2 \mathbf{f}_i &= \frac{\Delta \mathbf{f}_{i+1} - \Delta \mathbf{f}_i}{\Delta a_i} \quad (i = 1, \ldots, m-1), \end{aligned}$$

where $\Delta a_i = (\Delta s_i + \Delta s_{i+1})/2$ is the portion of arc length associated with vertex $\mathbf{f}_i$. We again denote by $\mathcal{C}_o$ the set of perturbations for $\mathbf{f}$ which preserve the endpoint values — $(m+1)$-vectors of vertices $\mathbf{h} \in (\mathbf{R}^n)^{m+1}$ such that $\mathbf{h}_0 = \mathbf{h}_m = \mathbf{0}$. The discretized curve length is then

$$\phi(\mathbf{f}) = \sum_{i=1}^{m} \Delta s_i, \tag{25.6}$$

and the ordinary gradient $\nabla \phi(\mathbf{f}) \in \mathcal{C}_o$ has component n-tuples

$$\nabla \phi_i = \frac{\partial \phi}{\partial \mathbf{f}_i} = \Delta \mathbf{f}_i - \Delta \mathbf{f}_{i+1},$$

for $i = 1, \ldots, m-1$. Note that $\nabla \phi_i = -\Delta a_i \Delta^2 \mathbf{f}_i$ so that the negative gradient at $\mathbf{f}_i$ has the direction of the normal curvature vector as in the continuous case (2). Again, critical points are characterized by zero curvature. Note also that the discretization of $\nabla \phi(f)$ as defined in (2) is $\nabla \phi_i = (\Delta \mathbf{f}_i - \Delta \mathbf{f}_{i+1})/\Delta t$, and hence the ordinary gradient of the discretized functional is not the discretized L_2 gradient. However, it has the same zeros (even when Δt_i is not constant).

Now define a discrete differential operator D_f by

$$(D_f \mathbf{h})_i \equiv \frac{\mathbf{h}_i - \mathbf{h}_{i-1}}{\sqrt{\Delta s_i}} \quad (i = 1, \ldots, m)$$

for $\mathbf{h} \in \mathcal{C}_o$. For $m = 4$, the matrix is

$$D_f = \begin{pmatrix} -1/\sqrt{\Delta s_1} & 1/\sqrt{\Delta s_1} & 0 & 0 & 0 \\ 0 & -1/\sqrt{\Delta s_2} & 1/\sqrt{\Delta s_2} & 0 & 0 \\ 0 & 0 & -1/\sqrt{\Delta s_3} & 1/\sqrt{\Delta s_3} & 0 \\ 0 & 0 & 0 & -1/\sqrt{\Delta s_4} & 1/\sqrt{\Delta s_4} \end{pmatrix},$$

and the negative Laplacian is

$$L_f \equiv D_f^T D_f = \begin{pmatrix} \frac{1}{\Delta s_1} & -\frac{1}{\Delta s_1} & 0 & 0 & 0 \\ -\frac{1}{\Delta s_1} & \frac{1}{\Delta s_1} + \frac{1}{\Delta s_2} & -\frac{1}{\Delta s_2} & 0 & 0 \\ 0 & -\frac{1}{\Delta s_2} & \frac{1}{\Delta s_2} + \frac{1}{\Delta s_3} & -\frac{1}{\Delta s_3} & 0 \\ 0 & 0 & -\frac{1}{\Delta s_3} & \frac{1}{\Delta s_3} + \frac{1}{\Delta s_4} & -\frac{1}{\Delta s_4} \\ 0 & 0 & 0 & -\frac{1}{\Delta s_4} & \frac{1}{\Delta s_4} \end{pmatrix},$$

where L_f is applied to an element $\mathbf{h} \in \mathcal{C}_o$ by applying it to each of the n $(m+1)$-vectors associated with the components. If components of $\mathbf{h}$ are stored contiguously, the zeros and ones in L_f may be interpreted as order-n matrices. L_f approximates a Neumann Laplacian, and has the constant vectors in its null space. We restrict L_f to $\mathcal{C}_o$ and follow its application with projection onto $\mathcal{C}_o$ by simply omitting the first and last columns, and the first and last rows, respectively. Then we have a symmetric positive-definite tridiagonal matrix $P_o L_{f|\mathcal{C}_o}$ which we use in the discrete version of (5) to compute the Sobolev gradient. Note that we solve n linear systems with the same order-$(m-1)$ matrix. The following theorem shows that, as in the continuous case, one step of steepest descent with the Sobolev gradient and step-length 1 produces the solution.

Theorem 25.3. *For any discrete curve* $\mathbf{f}$, $\mathbf{f} - (P_o L_{f|\mathcal{C}_o})^{-1} \nabla \phi(\mathbf{f})$ *is a parametric line segment with endpoints* $\mathbf{f}_0$ *and* $\mathbf{f}_m$ *and with the same vertex distribution as the initial curve* f.

Proof. Let $\mathbf{l} = \mathbf{f} - (P_o L_{f|\mathcal{C}_o})^{-1} \nabla \phi(\mathbf{f})$. Then $\nabla \phi(\mathbf{f}) = (P_o L_{f|\mathcal{C}_o})(\mathbf{f} - \mathbf{l})$; i.e., for $i = 1, \ldots, m-1$,

$$\begin{aligned} \Delta \mathbf{f}_i - \Delta \mathbf{f}_{i+1} &= -\frac{1}{\Delta s_i}(\mathbf{f} - \mathbf{l})_{i-1} + \left(\frac{1}{\Delta s_i} + \frac{1}{\Delta s_{i+1}} \right) (\mathbf{f} - \mathbf{l})_i - \frac{1}{\Delta s_{i+1}} (\mathbf{f} - \mathbf{l})_{i+1} \\ &= \frac{(\mathbf{f} - \mathbf{l})_i - (\mathbf{f} - \mathbf{l})_{i-1}}{\Delta s_i} - \frac{(\mathbf{f} - \mathbf{l})_{i+1} - (\mathbf{f} - \mathbf{l})_i}{\Delta s_{i+1}} \\ &= \Delta \mathbf{f}_i - \Delta \mathbf{f}_{i+1} - \frac{\mathbf{l}_i - \mathbf{l}_{i-1}}{\Delta s_i} + \frac{\mathbf{l}_{i+1} - \mathbf{l}_i}{\Delta s_{i+1}}, \end{aligned}$$

and hence $(\mathbf{l}_{i+1} - \mathbf{l}_i)/\Delta s_{i+1} - (\mathbf{l}_i - \mathbf{l}_{i-1})/\Delta s_i = \mathbf{0}$. Thus, all segments of $\mathbf{l}$ are collinear, and $\|\mathbf{l}_{i+1} - \mathbf{l}_i\| / \|\mathbf{l}_i - \mathbf{l}_{i-1}\| = \|\mathbf{f}_{i+1} - \mathbf{f}_i\| / \|\mathbf{f}_i - \mathbf{f}_{i-1}\|$ for $i = 1, \ldots, m-1$. □

The Hessian of ϕ at $\mathbf{f}$ is the block tridiagonal matrix with the following order-n blocks in row i:

$$H_{i,i-1} = \frac{\partial^2 \phi}{\partial \mathbf{f}_i \partial \mathbf{f}_{i-1}} = -\frac{I - \Delta \mathbf{f}_i \mathbf{f}_i^T}{\Delta s_i}$$

$$H_{i,i} = \frac{\partial^2 \phi}{\partial \mathbf{f}_i^2} = \frac{I - \Delta \mathbf{f}_i \mathbf{f}_i^T}{\Delta s_i} + \frac{I - \Delta \mathbf{f}_{i+1} \mathbf{f}_{i+1}^T}{\Delta s_{i+1}}$$

$$H_{i,i+1} = \frac{\partial^2 \phi}{\partial \mathbf{f}_i \partial \mathbf{f}_{i+1}} = -\frac{I - \Delta \mathbf{f}_{i+1} \mathbf{f}_{i+1}^T}{\Delta s_{i+1}}$$

for $i = 1, \ldots, m-1$. It is easily verified that $H(\mathbf{f}) = D_f^T P D_f$, where P is a block diagonal matrix with blocks $P_i = I - \Delta \mathbf{f}_i \Delta \mathbf{f}_i^T$, and $H(\mathbf{f})$ is singular when $\mathbf{f}$ is a discretized line segment with constant unit tangent vector $\Delta \mathbf{f}$. Any sequence of vertices beginning and ending at the origin and lying on the line defined by $\Delta \mathbf{f}$ is an element of $\mathcal{C}_o$ and lies in the null space of $H(\mathbf{f})$ in this case.

The discrete version of the quadratic functional ψ is

$$\psi(\mathbf{f}) = (1/2\Delta t) \sum_{i=1}^{m} \Delta s_i^2,$$

where $\Delta t = 1/m$ is the time interval associated with each curve segment, assumed constant as mentioned in the opening paragraph of this section. Since this constant has no affect on critical points, we use the definition

$$\psi(\mathbf{f}) = \frac{1}{2} \sum_{i=1}^{m} \Delta s_i^2. \tag{25.7}$$

The gradient $\Delta \psi(\mathbf{f})$ has components

$$\Delta \psi_i = \frac{\partial \psi}{\partial \mathbf{f}_i} = -\mathbf{f}_{i-1} + 2\mathbf{f}_i - \mathbf{f}_{i+1},$$

and the Hessian of ψ is the block tridiagonal matrix ($m-1$ order-n blocks) with constant diagonal blocks $2I$ and off-diagonal blocks $-I$. This matrix is also proportional to the negative Dirichlet Laplacian $L = D^T D$, where D is the discrete first derivative operator defined by $(D\mathbf{h})_i = (\mathbf{h}_i - \mathbf{h}_{i-1})/\Delta t$. One Newton iteration produces a zero of $\nabla \psi$ characterized by $\mathbf{f}_{i+1} - \mathbf{f}_i = \mathbf{f}_i - \mathbf{f}_{i-1}$ for $i = 1, \cdots, m$.

25.4 Test Results

We tested three methods: steepest descent with the ordinary gradient, steepest descent with the discretized Sobolev gradient, and Newton's method, on the two problems: minimization of $\phi(\mathbf{f})$ and minimization of $\psi(\mathbf{f})$ defined by (6) and (7), respectively. In most cases we took the initial curve $\mathbf{f}$ to be a uniformly distributed sequence of $m = 200$ vertices on the parametric cubic spline interpolant of (0,0), (1,1), (0,1), and (1,0) in that order — a self-intersecting curve with endpoints (0,0) and (1,0).

For the most part, the test runs merely serve as dramatic illustrations of the theorems. The Sobolev gradient method produces the discretized line segment (with accuracy close to machine precision) in a single iteration, as does Newton's method for minimizing ψ. Newton's method applied to ϕ failed to converge even when started with an initial estimate very close to the line segment. The most interesting result was the miserable performance of the standard method of steepest descent. For minimizing ϕ the method failed (was unable to further reduce the functional) far from the solution, both with a line search and with a small constant step-size (0.01). When applied to the quadratic functional ψ, the method converged to a line segment of length 1.001 but only with constant step-size at most 0.5, and that required 39000 iterations in the best case.

The problem treated here is very special in that, by Theorem 3.1, the solution of a linear system (inverting the **f**-Laplacian) essentially produces the solution of a system of nonlinear equations $\nabla\phi(\mathbf{f}) = \mathbf{0}$. On the other hand, the relative effectiveness of the Sobolev gradient method compared to a gradient descent method with the ordinary gradient is not atypical. Our experience with more challenging geometric problems is that the standard gradient descent methods fail completely due to the lack of smoothness in the discretized L_2 gradient while the Sobolev gradient method requires very few iterations for convergence — at most a few hundred, and often fewer than 10.

Chapter 26
Numerical Differentiation, Sobolev Gradients

R. Wallace and I. Knowles

26.1 Introduction

Consider the problem of determining, numerically, the values of the derivative of an underlying function, such as the one illustrated below, when we only know values of the function that have been perturbed by some kind of uniform error. Functions such as these arise frequently in scientific applications, generally as a result of the inherent errors present in measurement processes. If one were to attempt to use standard numerical techniques, such as the central difference formula, to compute approximated derivative values for the underlying function, it is evident that the errors in these derivatives would greatly exceed the measurement error present in the original function data. In fact, it has long been known that with no restrictions on the type of uniform perturbation that one allows, one can construct examples in which the difference between the original and perturbed derivative values is arbitrarily large.

The real problem from a practical standpoint therefore is this: assuming some kind of uniform perturbation, one seeks to delineate a class of suitable perturbations, with the intention of being able to compute, within the class, an approximate derivative whose magnitude of error is approximately that of the original uniform perturbation. The "suitable class " here would typically depend on the application, but is generally clear in specific cases.

Our task now is to present an approach to these problems that is variational in nature. More precisely, we compute the desired approximate derivative by minimizing a functional. As we see presently, the "suitable class" mentioned above turns out to be the set of all solutions of Sturm-Liouville boundary value problems defined on a given fixed interval of the real line; this class is large, and generally quite relevant in practical applications.

Given a discrete set of function values, such as those one might obtain from some scientific measurement process, one can always use, for example, spline interpolation to obtain a C^2 function u defined on some closed interval $[a, b]$; the graph of this u would typically be irregular, but smooth, and likely look something like that of Figure 26.1. We seek to compute an approximation

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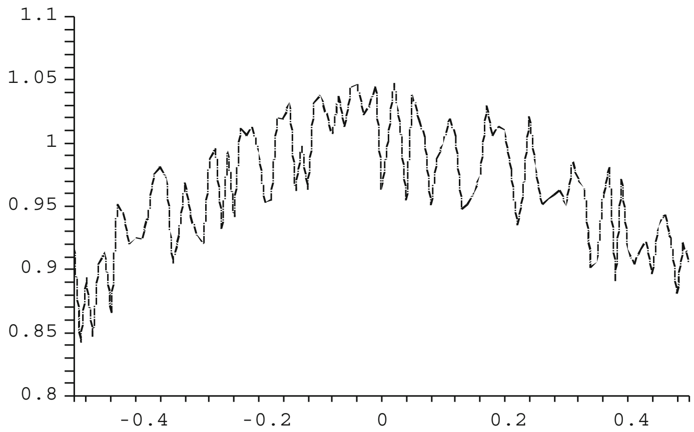


Fig. 26.1 A function with error

to the derivative of the underlying unperturbed function represented by the data. By adding a suitable constant if necessary, we can assume without loss of generality that $u > 0$. Set $A = u(a)$ and $B = u(b)$. If we define $Q(x) = u''(x)/u(x)$ for all x in $[a, b]$ then it is clear that the function u satisfies the Sturm-Liouville boundary-value problem

$$\begin{aligned} -u'' + Q(x)u &= 0, \\ u(a) = A, \qquad u(b) &= B. \end{aligned} \tag{26.1}$$

This formulation now allows us to recast numerical differentiation as an inverse problem. Specifically, we are given the solution u of a Sturm-Liouville equation, and we seek to recover the coefficient function Q; in so doing, we are in reality determining the second derivative u'', from which process it will not be difficult to extract the first derivative u' that we seek.

The specific inverse technique that we use here involves the construction of an associated functional H defined by

$$H(q) = \int_a^b (u'^2 + qu^2)\, dx - \int_a^b (u_q'^2 + qu_q^2)\, dx, \tag{26.2}$$

where u_q solves the boundary value problem

$$\begin{aligned} -v'' + q(x)v &= 0, \\ v(a) = A, \quad v(b) &= B. \end{aligned} \tag{26.3}$$

We show below that the functional H is strictly convex, and has a unique global minimum, $Q = u''/u$, that may be obtained approximately using a steepest descent technique. Once an approximation to Q is found, we obtain an approximation for u' by numerically solving $-u'' + Q(x)u = 0$ as a first order system under appropriate boundary conditions. The use of a Sobolev space gradient for H, rather than the more common $\mathcal{L}^2$-gradient, is a crucial step in our development. We note in passing that the fact that the formula for H contains the sought-after derivative u' is not an issue because, as we show below in Proposition 26.2(e), the formula for the differences $H(q_1) - H(q_2)$ does not involve u', and this is all that we need to execute the descent process.

The precise form of the functional H given in (26.2) has an interesting, if rather circuitous, history. Following a suggestion of John Neuberger, we were exploring how one might solve inverse problems "variationally". We knew that, from the Dirichlet principle, the Dirichlet energy functional is minimized to obtain solutions of selfadjoint elliptic problems, and so the general idea was to find an "inverse Dirichlet principle", i.e. to use something like the Dirichlet energy functional to find the coefficient functions in an elliptic problem, given the solution. The simplest equation of this type is

$$-\left(P(x)u'\right)' = 0, \quad u(a) = A, u(b) = B, \tag{26.4}$$

where u is presumed known, and $P > 0$ is to be determined. One might now try to obtain P by minimizing the Dirichlet form

$$D(p) = \int_a^b p(x)u'(x)^2\,dx$$

with respect to p, in some sense. This version however is quickly seen to be doomed at the outset because, for a given u, (26.4) is satisfied by all multiples of P, so the inverse problem does not have a unique solution, at least if stated in this form.

To counter this "multiplier" problem, we then considered minimizing $D(p)$ under the constraint condition on p that

$$\int_a^b p(x){u_p'}^2\,dx = \int_a^b P(x)u'^2\,dx,$$

where u_p is the solution of (26.4) with P replaced by p; a short argument using the Dirichlet principle showed that P was indeed the minimum here. In the case of equation (26.1) now, the analogous idea is that we are given u and we minimize

$$D(q) = \int_a^b (u'(x))^2 + q(x)u^2(x)\,dx$$

subject to the constraint that

$$\int_a^b {u_q'}^2 + q(x){u_q}^2\,dx = \int_a^b u'^2 + Q(x)u^2\,dx.$$

If one uses a Lagrange multiplier argument to convert the constrained minimization to an unconstained one, setting the Lagrange multiplier variable equal to one in the process, then H appears as the relevant functional for the unconstrained process.

In Section 26.2 we investigate the functional H, and the stability of the optimization process is examined in Section 26.3. A Steepest Descent Algorithm is outlined in Section 26.4, and some numerical examples are considered in Section 26.5. The present account summarizes and updates earlier work presented in [102].

26.2 The Functional $H(q)$

Given that the Sturm-Liouville equation (26.1) has a positive solution, it must be disconjugate on the interval $[a, b]$, i.e. every non-trivial solution can have at most one zero on this interval (see [46, pp. 1, 5]). The importance of disconjugacy in the present context is that this condition is necessary and sufficient [79, p. 351] for the solubility of Sturm-Liouville boundary problems like (26.3). With this in mind, we define $\mathcal{D}$ to be the set of all functions q in $\mathcal{L}^1[a, b]$ such that the equation (26.3) is disconjugate on $[a, b]$. It follows from [46, pp. 10, 95] that $\mathcal{D}$ is convex and open in both $\mathcal{L}^1[a, b]$ and $\mathcal{L}^2[a, b]$, and we note in passing that for $q \in \mathcal{D}$, each solution u_q of (26.3) is positive, as each of A and B is positive by assumption. Note also that $Q \in \mathcal{D}$. For technical reasons that will become clear presently, we need to assume in the sequel that

$$\|Q\|_\infty \le M, \tag{26.5}$$

where

$$0 < M < \frac{\pi^2}{(b-a)^2}. \tag{26.6}$$

Conditions (26.5) and (26.6) serve to control the curvature of the function u in that more curvature is permitted with $b - a$ small.

For each $q \in \mathcal{D}$, let the associated homogeneous Dirichlet operator A_q be defined by $A_q v = -v'' + qv$; this operator acts on functions v in the Sobolev space $\mathcal{H}^2[a, b]$ satisfying homogeneous Dirichlet boundary conditions at the end points of the interval $[a, b]$. In addition, let G_q be the Green's function associated with the operator A_q. Recall that G_q is continuous, hence bounded, on $[a, b] \times [a, b]$. We use $\|\cdot\|_p$ to denote the usual norms in the spaces $\mathcal{L}^p[a, b]$, $1 \le p \le \infty$.

Lemma 26.1. *For fixed q in $\mathcal{D}$ and h in $\mathcal{L}^1[a,b]$ such that*

$$\|h\|_1 < \frac{1}{2}\|G_q\|_\infty^{-1}, \tag{26.7}$$

we have the following estimates:

$$\|u_{q+h}\|_\infty \le 2\|u_q\|_\infty; \tag{26.8}$$

$$\|u_{q+h} - u_q\|_\infty \le 2\|G_q\|_\infty \|u_q\|_\infty \|h\|_1. \tag{26.9}$$

Proof. Subtracting the equations $-u''_{q+h} + (q+h)u_{q+h} = 0$ and $-u''_q + qu_q = 0$, and observing that $u_{q+h} - u_q$ lies in the domain of the operator A_q, we obtain $A_q(u_{q+h} - u_q) = -hu_{q+h}$. As q is in $\mathcal{D}$, the operator A_q is positive [79, p. 352], and hence it may be inverted; thus

$$u_{q+h}(x) = u_q(x) - \int_a^b G_q(x,\xi)u_{q+h}(\xi)h(\xi)\,d\xi. \tag{26.10}$$

Consequently, $|u_{q+h}(x)| \le \|u_q\|_\infty + \|G_q\|_\infty\|u_{q+h}\|_\infty\|h\|_1$ for all $a \le x \le b$. From (26.7) $\|u_{q+h}\|_\infty \le \|u_q\|_\infty + \|G_q\|_\infty\|u_{q+h}\|_\infty\|h\|_1 \le \|u_q\|_\infty + \frac{1}{2}\|u_{q+h}\|_\infty$, and (26.8) follows.

To see that (26.9) holds observe that from (26.10) one readily obtains

$$|u_{q+h}(x) - u_q(x)| \le \|G_q\|_\infty\|u_{q+h}\|_\infty\|h\|_1$$

for $a \le x \le b$. By taking the maximum of the left side over $a \le x \le b$ and applying (26.8) to the right side we have (26.9), whenever (26.7) holds. □

We next gather together some of the more useful properties of the functional H.

Proposition 26.2. *(a) $H(q) \ge 0$ for q in $\mathcal{D}$, and $H(q) = 0$ if and only if $q = Q$.*

(b) The Fréchet differential H' is given by

$$H'(q)h = \int_a^b (u^2 - u_q^2)h\,dx$$

for all q in $\mathcal{D}$ and h in $\mathcal{L}^1[a,b]$, and the $\mathcal{L}^2$-gradient of H is given by $\nabla H(q) = u^2 - u_q^2$.

(c) The second Fréchet differential of H is given by

$$H''(q)[h,k] = 2\left(A_q^{-1}(u_q h), u_q k\right)$$

for each q in $\mathcal{D}$ and h,k in $\mathcal{L}^1[a,b]$; further, for each such q the quadratic form $H''(q)$ is positive definite, and the functional H is strictly convex.

(d) For any q in $\mathcal{D}$,

$$H(q) = \int_a^b [(u' - u_q')^2 + q(u - u_q)^2]\, dx.$$

(e) For any q_1, q_2 in $\mathcal{D}$,

$$H(q_1) - H(q_2) = \int_a^b (q_1 - q_2)(u^2 - u_{q_1} u_{q_2})\, dx.$$

Proof. (a) To see that the first property holds, note that $u = u_Q$ and by Dirichlet's principle applied to the boundary value problem (26.3),

$$\int_a^b (u'^2 + qu^2)\, dx \geq \int_a^b (u_q'^2 + qu_q^2)\, dx,$$

with equality if and only if $u = u_q$. Hence $H(q) \geq 0$ for all q in $\mathcal{D}$, and $H(q) = 0$ if and only if $u_q = u_Q$; from the differential equations, the latter condition holds if and only if $(q - Q)u = 0$, and the desired result follows from the positivity of u.

(b) For h in $\mathcal{L}^1[a, b]$ let $I(h)$ be given by

$$I(h) = H(q + h) - H(q) - \int_a^b (u^2 - u_q^2) h\, dx.$$

Using the definition of H, integration by parts, the equations for u_q and u_{q+h}, and the fact that u_q and u_{q+h} agree on the boundary of $[a, b]$, we have that

$$\begin{aligned} I(h) &= \int_a^b [-(u_q''+u_{q+h}'') + q(u_q + u_{q+h})](u_q - u_{q+h})\, dx + \int_a^b (u_q^2 - u_{q+h}^2) h\, dx \\ &= \int_a^b (u_q - u_{q+h}) u_q h\, dx. \end{aligned}$$

Then (26.9) yields

$$|I(h)| \leq \|u_q - u_{q+h}\|_\infty \|u_q\|_\infty \|h\|_1 \leq 2\|G_q\|_\infty \|u_q\|_\infty^2 \|h\|_1^2,$$

whenever (26.7) holds. Property (b) then follows by Taylor's theorem. (c) For fixed k in $\mathcal{L}^1[a, b]$ define

$$J(h) = H'(q + h)k - H'(q)k - 2 \int_a^b \int_a^b G_q(x, \xi) u_q(x) u_q(\xi) k(x) h(\xi)\, d\xi dx.$$

Then, by using the expression for H' given in part (b), we see that

$$\begin{aligned}J(h) &= \int_a^b (u_q^2 - u_{q+h}^2)k\,dx - 2\int_a^b\int_a^b G_q(x,\xi)u_q(x)u_q(\xi)k(x)h(\xi)\,d\xi dx.\\ &= \int_a^b [u_q(x)+u_{q+h}(x)]k(x)\int_a^b G_q(x,\xi)u_{q+h}(\xi)h(\xi)\,d\xi dx\\ &\quad -2\int_a^b\int_a^b G_q(x,\xi)u_q(x)u_q(\xi)k(x)h(\xi)\,d\xi dx,\end{aligned}$$

upon factoring the first integrand and then using (26.10) to eliminate $u_q - u_{q+h}$. Estimating as before, we see that $|J(h)| \le 8\|G_q\|_\infty^2\|u_q\|_\infty^2\|h\|_1^2\|k\|_1$, whenever (26.7) holds. Hence

$$\begin{aligned}H''(q)[h,k] &= 2\int_a^b\left(\int_a^b G_q(x,\xi)u_q(\xi)h(\xi)\,d\xi\right)u_q(x)k(x)\,dx\\ &= 2(A_q^{-1}(u_qh), u_qk),\end{aligned}$$

as required. Finally, notice that $H''(q)[h,h] = 2(y, A_q y)$, where $A_q y = u_q h$. As A_q is positive, y is the trivial solution if and only if $u_q h$ (and hence h) is the zero function, and thus we have that, for each q in $\mathcal{D}$, $H''(q)$ is a positive definite form. It follows from this that H is strictly convex on $\mathcal{D}$. (d) Note that, on rearranging (26.2),

$$\begin{aligned}H(q) &= \int_a^b (u'^2 - 2u'u_q' + u_q'^2)\,dx\\ &\quad + \int_a^b q(u^2 - 2uu_q + u_q^2)\,dx + 2\int_a^b [(u'-u_q')u_q' + q(u-u_q)u_q]\,dx.\end{aligned}$$

Further, integration by parts shows that

$$\int_a^b [(u'-u_q')u_q' + q(u-u_q)u_q]\,dx = (u-u_q)u_q'|_a^b + \int_a^b (-u_q'' + qu_q)(u-u_q)\,dx,$$

which is clearly zero, as u and u_q agree at the endpoints of $[a,b]$ and u_q is a solution of (26.3); property (d) now follows.

(e) Observe that after applying the definition of H and rearranging terms

$$\begin{aligned}&H(q_1) - H(q_2)\\ &= \int_a^b (u_{q_2}'^2 + q_1u_{q_2}^2)\,dx - \int_a^b (u_{q_1}'^2 + q_1u_{q_1}^2)\,dx + \int_a^b (u^2 - u_{q_2}^2)(q_1-q_2)\,dx,\end{aligned}$$

$$= \int_a^b [(u'_{q_1} - u'_{q_2})^2 + q_1(u_{q_1} - u_{q_2})^2]\, dx + \int_a^b (u^2 - u_{q_2}^2)(q_1 - q_2)\, dx,$$
$$= \int_a^b [-(u''_{q_1} - u''_{q_2}) + q_1(u_{q_1} - u_{q_2})](u_{q_1} - u_{q_2}) dx + \int_a^b (u^2 - u_{q_2}^2)(q_1 - q_2) dx,$$

by a computation similar to that used to prove property (d) above, as u_{q_1} and u_{q_2} agree on the boundary of $[a, b]$. Replacing u''_{q_1} and u''_{q_2} by $q_1 u_{q_1}$ and $q_2 u_{q_2}$, respectively, and combining like terms, completes the proof. □

26.3 Stability

It is clear from Proposition 26.2 that one can in theory recover $Q = u''/u$ by minimizing the convex functional H. We next examine precisely how perturbations in u, the function to be differentiated, affect the computed value of the derivative.

Let $\tilde{u} = u + \Delta$, where Δ is uniformly small and where $\Delta(a) = \Delta(b) = 0$. It is known that, with no further restrictions on Δ, $\|u' - \tilde{u}'\|_2$ can be arbitrarily large. We will show that by suitably restricting $\tilde{Q} = \tilde{u}''/\tilde{u}$, having Δ uniformly small, or $\tilde{u}'$ close to u' in $\mathcal{L}^2[a, b]$, or $H(\tilde{Q})$ small, are then all equivalent conditions.

Lemma 26.3. *Suppose that q is an $\mathcal{L}^1[a, b]$ function that satisfies*

$$\|q\|_\infty \le M, \tag{26.11}$$

where M satisfies (26.6). Then $q \in \mathcal{D}$ and $H(q) \ge \tau \|u - u_q\|^2_{\mathcal{H}^1}$, where

$$\tau = \frac{\frac{\pi^2}{(b-a)^2} - M}{1 + \frac{\pi^2}{(b-a)^2}} > 0. \tag{26.12}$$

Proof. Let h be in the Sobolev space $\mathcal{H}^1[a, b]$ with $h(a) = h(b) = 0$. Observe that by (26.11) we have

$$\int_a^b (h'^2 + qh^2) dx \ge \int_a^b (h'^2 - Mh^2)\, dx \ge \lambda_{-M} \int_a^b h^2\, dx, \tag{26.13}$$

where

$$\lambda_{-M} = \left[\frac{\pi^2}{(b-a)^2} - M \right]. \tag{26.14}$$

is the smallest eigenvalue of A_{-M}; so $q \in \mathcal{D}$ by [79, Theorem 6.2]. By (26.6), it follows that $0 < \tau < 1$. As we have from (26.12) and (26.14) that $(1 - \tau)$ $\lambda_{-M} - M\tau = \tau$,

$$\int_a^b (h'^2 - Mh^2)\,dx = (1-\tau)\int_a^b (h'^2 - Mh^2)\,dx + \tau\int_a^b (h'^2 - Mh^2)\,dx$$
$$\geq (1-\tau)\lambda_{-M}\int_a^b h^2\,dx + \tau\int_a^b h'^2\,dx - \tau M\int_a^b h^2\,dx$$
$$= \tau\int_a^b (h'^2 + h^2)\,dx. \tag{26.15}$$

Combining the first inequality in (26.13), and (26.15), and replacing h by $u - u_q$ yields, via Proposition 26.2(d), the desired result. □

Theorem 26.4. *Let u and Q be as defined above. Let $\tilde{u}$ be another positive twice differentiable function and let $\tilde{Q}$ be given by $\tilde{Q} = \tilde{u}''/\tilde{u}$. Suppose that $|Q(x)| \leq M$ and $|\tilde{Q}(x)| \leq M$ for $a \leq x \leq b$, where $0 < M < \pi^2/(b-a)^2$, and assume that $\tilde{u}(a) = u(a)$ and $\tilde{u}(b) = u(b)$. Then, with τ defined by (26.12),*

$$0 \leq \frac{1}{2M(b-a)^{3/2}||u||_\infty} H(\tilde{Q}) \leq (b-a)^{-\frac{1}{2}}||u-\tilde{u}||_\infty \leq ||u-\tilde{u}||_{\mathcal{H}^1} \leq \tau^{-1}H(\tilde{Q}).$$

Proof. By the previous lemma, $\tilde{Q}$ is in $\mathcal{D}$. So, by Proposition 26.2(e) we have that

$$H(\tilde{Q}) = \int_a^b (\tilde{Q} - Q)u(u - \tilde{u})\,dx,$$

as $H(Q) = 0$. The second inequality from the left in the theorem now follows. The inequality on the extreme right follows from Lemma 26.3. Also, as $\tilde{u}(a) = u(a)$, for all $x \in [a, b]$,

$$|u-\tilde{u}|(x) \leq \int_a^b |(u-\tilde{u})'(x)|\,dx \leq (b-a)^{1/2}\|(u-\tilde{u})'\|_2 \leq (b-a)^{1/2}\|u-\tilde{u}\|_{\mathcal{H}_1},$$

from which follows the remaining inequality. □

This estimate says that if we restrict our attention to the class of functions q that satisfy (26.11), then the problem of numerical differentiation by minimizing H (i.e. by making $H(\tilde{Q})$ as small as possible) becomes well-posed. The condition (26.11) serves as an upper bound on the allowable curvature of perturbations of the underlying function whose derivative is being sought.

26.4 Steepest Descent Minimization

Here we discuss the problem of minimizing the functional H, and estimating u' once a suitable approximation for the minimizer is found. As mentioned previously, our optimization strategy makes use of a steepest descent procedure.

First choose some initial function q_0 in $\mathcal{D}$ satisfying $\|q_0\|_\infty \le M$, where M is described by (26.6). Then from Proposition 26.2(a) the $\mathcal{L}^2$-direction of steepest descent for H at q_0 is $-\nabla H(q_0) = -(u^2 - u_{q_0}^2)$. However, there are significant numerical problems associated with using this gradient in the descent procedure. These stem from the fact that the $\mathcal{L}^2$-gradient is always zero on the boundary of $[a, b]$, as both u and u_q have the same boundary values. It follows that the boundary data for the evolving coefficient functions q are invariant during the descent; as this data is not known a priori, the consequences cannot be good. In practice, this approach leads to the presence of numerical solutions that exhibit severe decay near the boundary of the interval $[a, b]$ together with significant oscillation in the interior, as the algorithm attempts to do the best it can from the information in u.

One remedy for these problems is to use the Sobolev space gradient of H at q_0, $g_0 = \nabla_{\mathcal{H}^1} H(q_0)$, given by

$$H'(q_0)h = (g_0, h)_1$$

for all h in the Sobolev space $\mathcal{H}^1[a, b]$, where $(\cdot,\cdot)_1$ denotes the usual Sobolev inner product. One can readily show that g_0 is actually the solution of the Neumann boundary value problem $-v'' + v = \nabla H(q_0) = u^2 - u_{q_0}^2, v'(a) = v'(b) = 0$; in particular, if we write $g_0 = L^{-1}\nabla H(q_0)$ where L^{-1} is the integral operator obtained from the above Neumann problem, one can see that the $\mathcal{H}^1$-gradient is just a preconditioned (or, smoothed) $\mathcal{L}^2$-gradient. More importantly, one can see that the $\mathcal{H}^1$-gradient is allowed considerably greater freedom at the boundary, thus overcoming the difficulties discussed above.

The computation of boundary-value solutions like u_{q_0} is carried out using the method of invariant embedding [68, p. 117]. This allows us to convert the Sturm-Liouville boundary value problem

$$\begin{aligned} -v'' + q_0(x)v &= 0, \\ v(a) = A, \quad v(b) &= B, \end{aligned} \tag{26.16}$$

to a pair of initial-value problems. Specifically, let $z = v'$. Then (26.16) becomes

$$v' = z, \quad z' = q_0(x)v,$$

where $v(a) = A$ and $v(b) = B$. Let t solve the Ricatti-type initial-value problem

$$t' = q_0(x)t^2 - 1, \quad t(a) = 0,$$

and set $w = v + tz$. A short calculation shows that w satisfies

$$w' = q_0(x)tw, \quad w(a) = A,$$

and so (t, w) is now determined as the unique solution of a first order initial-value system. It follows that $z(b) = (w(b) - B)/t(b)$ is known. In order to counter the stiffness normally associated with the non-oscillatory Sturm-Liouville problem (26.16) we first set $r = v'/v$, and note from (26.16) that $r' = q_0 - r^2$; this equation is solvable on $[a, b]$, by [46, theorem 3]. We may now solve the final-value Ricatti system

$$r' = q_0 - r^2, \quad v' = rv,$$

backwards in x using the known values for $r(b) = z(b)/B$ and $v(b) = B$ to compute $v = u_{q_0}$ and $rv = u'_{q_0}$.

Note that the function $f_0(\alpha) = H(q_0 - \alpha g_0)$ is strictly decreasing in some right neighborhood of $\alpha = 0$ as $f_0'(0) = -\|g_0\|^2_{\mathcal{H}^1} < 0$. This function is now minimized by using a standard algorithm for the minimization of a function of one variable, such as that of Brent [182, §10.2], together with an appropriate "bracketing" algorithm (see [182, §10.1]), to find the local minimum $\alpha_0 > 0$. Then we set $q_1 = q_0 - \alpha_0 g_0$, and compute u_{q_1} and u'_{q_1} as above. This gives our first approximation:

$$u_{q_1} \approx u, \quad u'_{q_1} \approx u'.$$

This procedure is repeated with q_n replaced by $q_{n+1} = q_n - \alpha_n g_n$, for $n = 1, 2, \ldots$, where $g_n = \nabla_{\mathcal{H}^1} H(q_n)$, and α_n is chosen to locally minimize $f_n(\alpha) = H(q_n - \alpha g_n)$ in the manner described above, until H fails to descend. We use the identity given in Proposition 26.2(e) to monitor the descent. The convergence of this algorithm, under certain additional conditions, is established in [102, Theorems 5.1-2].

26.5 Some Numerical Examples

As a first example, we study the effect of roundoff error when a small stepsize, h, is used in the central difference discretization of a derivative. The effect of taking a small stepsize is known to severely amplify the effects of roundoff error, especially when the function to be differentiated is large compared to the value of the derivative [221, p. 145]. In fact, in the case of sufficiently small stepsize, the computed value of the derivative will be zero even when the correct value of the derivative is relatively large; see [221, Table 5.1]. Therefore, it is instructive to examine the computed derivative of $f(x) = \cos(x)$ at a value of x close, but not equal, to the stationary point $x = 0$. The results of such an experiment are given in Table 26.1. All computations are carried out using single precision floating point arithmetic. The function f is discretized on an interval with left endpoint $x = 0.001$, with a uniform mesh of stepsize h, and using the number of sub-intervals shown in the table. The derivative is calculated using the variational method discussed here and compared to values obtained using standard central differences. The large

Table 26.1 Relative error in computation of $f'(0.001)$, $f(x) = \cos x$

h	central difference	variational derivative	# subintervals	iterations
10^{-3}	0.0133	0.0004	100	3
10^{-4}	0.106	0.0013	100	6
10^{-5}	1.98	0.0729	500	1
10^{-6}	1.00	0.2847	500	2
10^{-7}	1.00	0.404	1000	1

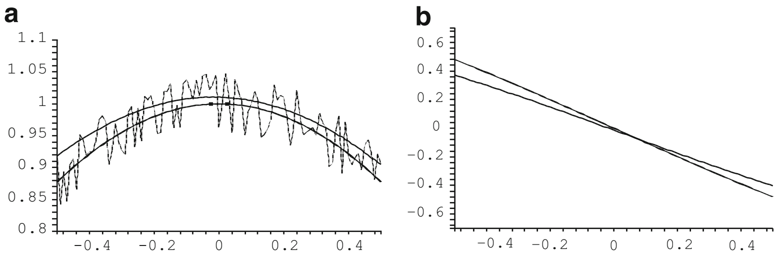
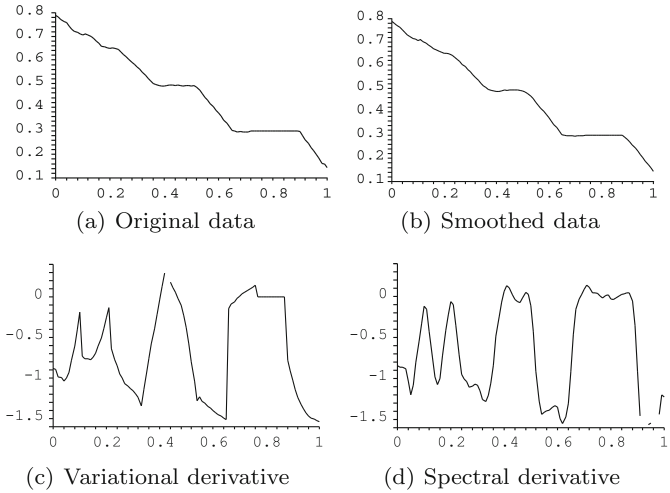


Fig. 26.2 Numerical differentiation of $\cos x + \epsilon(x)$, $|\epsilon(x)| \leq 0.05$

relative errors for the central difference method with $h \leq 10^{-5}$ indicate a complete breakdown of this method. It can be seen that the performance of the variational algorithm is close to optimal here. In particular, as the IEEE standard for single precision uses a 23 digit binary mantissa, and as $2^{-23} \approx 1.2 \times 10^{-7}$, the poor (but not disastrous) results for $h \leq 10^{-6}$ are probably as good as one could expect.

Next we examine the effect that a small random perturbation has on the variationally computed derivative. With $u(x) = \cos(x) + \varepsilon(x)$ for x in $[-0.5, 0.5]$, the values of $\varepsilon(x)$ are randomly chosen such that $|\varepsilon(x)| \leq 0.05$; see the irregular graph in Figure 26.2(a), and also Figure 26.1. We use the variational algorithm to numerically differentiate u using evenly spaced mesh points with $h = 10^{-2}$. The results are summarized in Figure 26.2 above. Here, the solid curves represent the underlying function, here $\cos x$, and its derivative, and the lighter curves in Figures 26.2(a) and (b) represent our variational approximation to the underlying function and its derivative, respectively. It can be seen from the latter that the error in the variationally computed derivative is of the same order of magnitude as the error in the given function; this is of course, optimal. We have observed that the variational method works best on small intervals. This is in agreement with the theory in that (26.6) shows that the estimated function q_n is more likely to be in the set $\mathcal{D}$ (and to satisfy (26.5)) when $b-a$ is small, so that the constant M may be large, if needed. For experimental data one is limited in how small $b - a$ may be chosen by the fact that too few data points in an interval tend to make the initial value solvers ineffective; in general one needs 5 to 10 data points per interval to avoid this problem.



(a) Original data (b) Smoothed data

(c) Variational derivative (d) Spectral derivative

Fig. 26.3 Differentiation of the Pallaghy-Lüttge data from plant physiology

The variational algorithm is also effective on practical data. We consider the differentiation of data on plant physiology experiments given in the paper [176] of Pallaghy and Lüttge. In this case the data function u is defined for 101 equally spaced x-values in $[0, 1]$, so that $h = 0.01$. From the comments above, it is prudent to divide the problem into ten sub-problems, each over a subinterval of length 0.1. The results are summarized in Figure 26.3 above, wherein Figure 26.3(a) represents the original Pallaghy-Lüttge data and Figure 26.3(c) represents the underlying numerical derivative obtained with the variational algorithm. As a by-product of the numerical differentiation procedure we are able to recover the data function almost exactly, as may be seen in Figure 26.3(b). By way of comparison, the alternative Fourier method of Anderssen and Bloomfield [4] applied to the same data gives rise to the numerical derivative shown in Figure 26.3(d).

26.6 Related Inverse Problems

The inverse technique employed above extends readily to higher dimensions. In particular, one can consider the problem of recovering the coefficient functions $P > 0$, $Q > 0$, and R in the selfadjoint elliptic equation

$$-\nabla \cdot P(x)\nabla u + \lambda Q(x)u = R(x), \tag{26.17}$$

over x in some bounded region $\Omega \subset \mathbb{R}^n$, from a knowledge of the solutions $u(x, \lambda)$. Inverse problems such as these arise frequently in applications. For example, in modelling groundwater flow in a two-dimensional region Ω it is common to use the groundwater flow equation

$$Q(x)\frac{\partial w}{\partial t} = \nabla \cdot P(x)\nabla w + \tilde{R}(x,t), \qquad x \in \Omega, \quad 0 \le t \le 1,$$

where $w(x,t)$ represents the water level at time t, for a well located at position x in the aquifer. Here, P represents the hydraulic conductivity of the subsurface, and Q the storativity, and $\tilde{R}$ represents the aquifer recharge term. All of these quantities are difficult to measure directly; it is however, relatively easy to monitor the aquifer water levels $w(x,t)$, albeit only at sparsely scattered values x. One easily obtains data for the elliptic equation (26.17) via the finite Laplace transform:

$$u(x,\lambda) = \int_0^1 w(x,t)e^{-\lambda t}\,dt.$$

We arrive then at a new problem: given $u(x,\lambda)$ satisfying (26.17) for $x \in \Omega$ and all $\lambda > 0$, and assuming, for uniqueness purposes, that P is known on the boundary of Ω, recover the functions P, Q, and R.

To this end, consider the functional $H(p,q,r,\lambda)$ given by

$$H(p,q,r,\lambda) = \int_\Omega p(x)|\nabla(u - u_{p,q,r,\lambda})|^2 + \lambda q(x)(u - u_{p,q,r,\lambda})^2\,dx,$$

where $v = u_{p,q,r,\lambda}$ is the unique solution of the boundary value problem

$$-\nabla \cdot (p(x)\nabla v(x,\lambda)) + \lambda q(x)v(x,\lambda) = r(x), \quad v|_{\partial\Omega} = u|_{\partial\Omega}.$$

One can see from Proposition 26.2(d) that the functional H here is an exact analogue of the earlier one. The key properties needed to establish the previous theory are that the associated Dirichlet operator be positive and selfadjoint, and that the Dirichlet principle, that forward solutions may be obtained by minimization, holds. Indeed, as noted earlier, in obtaining solutions of this inverse problem by minimization, we have in effect created a kind of inverse Dirichlet principle.

Notice that, in this setting $u = u_{P,Q,R,\lambda}$, where P, Q, and R are the functions that we seek. The Fréchet differential of H is given by

$$\begin{aligned} H'(p,q,r,\lambda)[h_1,h_2,h_3] = \int_\Omega &\left(|\nabla u|^2 - |\nabla u_{p,q,r,\lambda}|^2\right) h_1(x) \\ &+\lambda(u^2 - u_{p,q,r,\lambda}^2)h_2(x) - 2(u - u_{p,q,r,\lambda})h_3(x)\,dx. \end{aligned}$$

In this notation, the values of H' represent various directional derivatives for the functional H, with the functions h_1, h_2, and h_3 serving as the "directions" in which one might choose to vary p, q, or r, respectively.

The functional, G, that we actually minimize to recover the desired flow coefficients, is formed by choosing $n_{max} \geq 3$ unequal positive values λ_i, $1 \leq i \leq n_{max}$, of the λ-parameter, and then setting

$$G(p, q, r) = \sum_{i=1}^{n_{max}} H(p, q, r, \lambda_i).$$

This functional is again strictly convex, with a unique global minimum and stationary point at (P, Q, R). Steepest descent using $\mathcal{H}^1$-gradients may then be used to recover the coefficient functions P, Q and R [100, 101].

Chapter 27
Steepest Descent and Newton's Method and Elliptic PDE

John M. Neuberger

27.1 Introduction

We ultimately seek full knowledge of all solutions to semilinear elliptic partial differential equations (PDE) of the form

$$\begin{cases} \Delta u + f_s(u) = 0 \text{ in } \Omega \\ B(u, \frac{\partial u}{\partial \eta}) = 0 \text{ on } \partial\Omega, \end{cases} \tag{27.1}$$

where Ω is a region in $\mathbb{R}^n$ and B enforces a given boundary condition (BC). Our methods apply immediately when f_s satisfies a superlinear hypothesis such as that found in [3, 34, 127–129] and B gives the standard Dirichlet or Neumann BC. For convenience, we take $f_s : \mathbb{R} \to \mathbb{R}$ to be defined here by $f_s(u) = su + u^3$, with s a real bifurcation parameter, unless otherwise specified. Observe that $f_s(0) = 0$ and $f_s'(0) = s$; the first fact implies that $u = 0$ is a solution for all s, whereas the second gives us an easy way to vary $f_s'(0)$ and obtain a bifurcation diagram. Analysis and key components of our algorithms use an orthonormal basis of eigenvectors of $-\Delta$, denoted by $0 = \lambda_1 < \lambda_2 \leq \cdots$ and $\{\psi_j\}$, respectively.

We would like accurate approximations of all lower energy, lower Morse index (MI) solutions, as well as geometric, variational, and topological information about them. We will present the mountain pass algorithm (MPA) and modified mountain pass algorithm (MMPA) from [127] for computing MI 1 and MI 2 solution approximations to our superlinear elliptic boundary value problem (BVP), where all nontrivial solutions are saddle points. In these algorithms Sobolev gradient descent is used in conjunction with steepest ascent to find a nontrivial solution u as a constrained minimum and a zero of the gradient of the functional $J_s : H \to \mathbb{R}$ defined by $J_s(u) = \int_\Omega \frac{|\nabla u|^2}{2} + F_s(u)$, where $F_s(t) = \int_0^t f_s$ and, if enforcing zero Dirichlet BC, H is the Sobolev space $H_0^{1,2}(\Omega)$.

In seeking higher MI solutions, we find that Newton's method in this setting can be viewed as performing steepest ascent on J_s in finitely many directions, while following steepest descent in all other directions. We will

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present the gradient Newton-Galerkin algorithm (GNGA) from [130, 131], and two variants from [132], the tangent-augmented GNGA and the cylinder-augmented GNGA. Our implementations of Newton's method enforce constraints which allow us to easily follow bifurcation curves and force branch switching at bifurcation points.

We currently use these algorithms to find many solutions of (27.1). In this recent research, symmetry has been an important consideration, in particular as a means of making our algorithms more efficient and robust. We only give a brief hint in this chapter concerning the role of symmetry in our applications, instead referring the reader to [128–132] and references therein. We will present an example result where Ω is a region bounded by the fractal Koch's snowflake.

Although we are interested in PDE, in discretizing equations such as (27.1) over some grid for the region Ω, one in fact is working with a discrete nonlinear system of equations. If one eliminates scaling and considers the graph Laplacian on a graph G, the resulting partial *difference* equation (PdE)

$$-Lu + f_s(u) = 0 \tag{27.2}$$

can be studied as an object of interest in its own right. This naturally leads to considering the symmetry of the graph G and all possible symmetries of solutions u. The reader is again referred to [127,132] and references therein for more details considering the symmetry aspect of this problem. We will present in this chapter an outline of our methodology and some example results whereby we find solutions as critical points of a functional $J_s : \mathbb{R}^n \to \mathbb{R}$ where $-\nabla J_s(u) = -Lu + f_s(u)$. The eigenvalues and corresponding eigenvectors of L are denoted by $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ and $\{\psi_j\}_{j=1}^n$, respectively. Much is known about the spectrum of the graph Laplacian. See, for example, [13, 23, 44].

Our first paper in this subject area [128] contains a fairly thorough list of citations relevant to the study of solutions to linear and nonlinear PdE. Most of the relevant literature concerns linear problems and/or positive solutions, whereas we are interested in the existence and symmetry of all solutions, in particular sign-changing ones, to nonlinear PdE.

27.2 The Variational Formulation for PDE and PdE

Let $f_s : \mathbb{R} \to \mathbb{R}$ be defined by our choice $f_s(u) = su + u^3$, or otherwise satisfy the hypothesis from [3, 34, 127–129]. If we consider, for example, zero Dirichlet boundary conditions, then solutions to (27.1) are critical points of the functional $J_s : H \to \mathbb{R}$ defined by

$$J_s(u) = \int_\Omega \frac{|\nabla u|^2}{2} - F_s(u).$$

Similarly, in seeking solutions to (27.2), we look for critical points of the function $J_s : \mathbb{R}^n \to \mathbb{R}$ defined by

$$J_s(u) = \frac{1}{2} Lu \cdot u - \sum F_s(u_i).$$

For steepest descent in the Sobolev space H, we integrate by parts and compute the gradient from

$$J_s'(u)(v) = \int_\Omega \nabla u \cdot \nabla v - f_s(u)v = \langle u - (-\Delta)^{-1} f_s(u), v \rangle_H = \langle \nabla J_s(u), v \rangle_H.$$

Solving the discretized sparse linear system for $-\Delta w = f_s(u)$ to get an accurate discretized approximation for $\nabla J_s(u) = u + w$ is a standard exercise in numerical analysis.

In [34] it is proven that there exists a sign-changing exactly-once MI 2 solution w_3 to (27.1), under our fairly standard superlinear hypothesis with also $f_s'(0) < \lambda_1$. For convenience, we call such functions CCN solutions. There, the C^1 Nehari manifold

$$S = \{u \in H | J'(u)(u) = 0, u \neq 0\} \text{ and its subset } S_1 = \{u \in S | u_+, u_- \in S\}$$

satisfy $J_s(w_3) = \min_{S_1} J_s$. For our superlinear hypothesis, points on S maximize J_s in every ray direction, like the rim of a volcano with the trivial solution being the minimum in the crater. The set S_1 separates positive and negative elements like an equator of S, which is diffeomorphic to the unit sphere in H. In [35], the existence result was extended for $f_s'(0) < \lambda_2$. For $s > \lambda_1$ the set S has 0 as a limit point and fails to be a manifold there. As in [3], the hypothesis also gives the existence of a positive solution w_1 and negative solution w_2, both MI 1 local minima of $J_s|_S$, provided $f_s'(0) < \lambda_1$. Steepest descent in H together with ascent on to S or S_1 are the MPA and MMPA, respectively. The effectiveness of these algorithms is a consequence of our proper choice of gradient.

Finding higher MI solutions and varying the parameter s requires more than the one or two constraints used in the MPA and MMPA. For a MI k solution, the Hessian $D^2 J_s(u)$ has k negative eigenvalues. With $\{\beta_i\}$ and $\{e_i\}$ the eigenvalues and eigenfunctions of the Hessian, we have

$$(D^2 J_s(u))^{-1} \nabla J_s(u) = \sum \frac{1}{\beta_i} P_{e_i} \nabla J_s(u).$$

Thus Newton's method of iterating

$$u_{j+1} = u_j - (D^2 J_s(u))^{-1} \nabla J_s(u)$$

in function space is in fact performing steepest ascent in the k directions where $\beta_i < 0$, and descent in the infinitely many other directions corresponding to positive eigenvalues of the Hessian. It is convenient that, where all quantities are defined, the term $(D^2 J_s(u))^{-1} \nabla J_s(u)$ is independent of whether the H or L_2 inner product is used. Thus, unlike Sobolev gradient descent/ascent (which would correspond to replacing $\frac{1}{\beta_i}$ with ± 1), we may use L_2 gradients and Hessians and expect good performance.

There are several approaches towards implementing this iteration numerically; all use discretization to reduce the problem to a finite dimension. The GNGA works in coordinate space using a suitable basis of eigenfunctions of the Laplacian for a subspace $A = \text{span}\{\psi_{i_j}\}_{j=1,\ldots,m}$ of H. Discretizing in Ω leads to a sparse $n-$dimensional linear system approximating

$$-\Delta u = \lambda u,$$

with boundary conditions. Standard tools such as ARPACK [107] are quite good at generating the first m or more eigenvectors if they are not known in closed form, although making an advantageous choice of basis vectors is an intricate matter if symmetry is to be used [130–132]. Essentially, we project eigenvectors corresponding to multiple eigenvalues on to fixed point spaces according to the fundamental isotypic decomposition and then perform the Gram-Schmidt orthonormalization process. For convenience, we write $\{\psi_j\}_M$ for the ultimate orthonormal basis selection.

Thus, when we say $(a, s) \in \mathbb{R}^{m+1}$ is a solution we mean that

$$u = \sum_{j=1}^{m} a_j \psi_j \in \mathbb{R}^n$$

satisfies $P_A \nabla J_s(u) = 0$. If n and m are small, it is reasonable to expect accurate approximations only for low MI, low J value solutions of (27.1) with parameter s. With the eigenvalues and eigenvectors in A in hand, we compute the gradient coordinate vector $g = g_s(u) \in \mathbb{R}^m$ by

$$g = (J_s'(u)(\psi_j))_m = (\lambda_j a_j - \int_\Omega f_s(u)\psi_j)_m, \tag{27.3}$$

where any of several standard numerical integration methods can be used in the nonlinear term. We have $P_A \nabla J_s(u) = \sum_m g_j \psi_j$, so we seek $g = 0 \in \mathbb{R}^m$. Similarly, the Hessian matrix $h = h_s(u)$ can be computed as

$$h = (J_s''(u)(\psi_j, \psi_k))_{m,m} = (\lambda_j \delta_{jk} - \int (f_s'(u))\psi_j \psi_k)_{m,m}, \tag{27.4}$$

where δ_{jk} is the Kronecker delta.

We define the signature $\mathrm{sig}(u,s)$ to be the number of negative eigenvalues of the matrix $h_s(u)$ representing the self-adjoint bilinear operator $D^2J_s(u)$. If (u,s) is a non-degenerate solution to (27.2), then $\mathrm{sig}(u,s)$ equals the Morse index $\mathrm{MI}(u,s)$. Non-invertible Hessians inevitably occur at bifurcation points and fold points (points where the solution branch is not monotonic in s). When the Hessian is singular, the subspace of eigenvectors of the Hessian with eigenvalue 0 is called the critical eigenspace, and is denoted by E. Symmetry can be used to decompose E into symmetry invariant component subspaces. It is efficient and robust to solve for search directions in these lower dimensional subspaces when seeking solutions on new branches near bifurcation points.

The operator ∇J_s is $\mathrm{aut}(\Omega)$-equivariant, i.e., $\nabla J_s(\alpha u) = \alpha \cdot \nabla J_s(u)$ for all $\alpha \in \mathrm{aut}\,(\Omega)$. Furthermore, if f_s is odd, then ∇J_s is $\Gamma_0 = \mathrm{aut}\,(G) \times \mathbb{Z}_2$-equivariant. If u is a solution to Equation (27.1) or (27.2) with f_s odd, then $\gamma{\cdot}u$ is also a solution to (27.1) for all $\gamma \in \Gamma_0$. Following the standard treatment [75, 131, 132], for each $\Gamma_i \leq \Gamma_0$ we define the fixed point subspace of the Γ_0 action on $V = \mathbb{R}^n$ to be

$$\mathrm{Fix}\,(\Gamma_i, V) = \{u \in \mathbb{R}^n \mid \gamma \cdot u = u \text{ for all } \gamma \in \Gamma_i\}.$$

These fixed point subspaces are ∇J_s-invariant. It is beyond the scope of this chapter to say much more, but if we take full advantage of knowledge of symmetry we can reduce the dimension of the costly computations for h to smaller fixed point spaces and perform intelligent branch switching at bifurcation points.

For PdE (27.2) on a graph G the variational equations are similar. The Laplacian of G is determined by the matrix L defined by letting $L_{ii} = d(v_i)$, $L_{ij} = -1$ if $\{v_i, v_j\} \in E_G$, and $L_{ij} = 0$ if $i \neq j$ but $\{v_i, v_j\} \notin E_G$, where $\{v_i\}$ are the n vertices of G and E_G is the corresponding set of edges. Up to scaling, if G come from a suitable grid, solutions to this PdE (27.2) approximate solutions to PDE (27.1) with zero Neumann boundary BC. Other BC can be explored by modifying L. The critical points of the functional

$$J_s(u) = Lu \cdot u - \sum_n F_s(u_i)$$

are solutions to PdE (27.2). Here, the gradient vector satisfies

$$g_j = \lambda_j a_j - f_s(u) \cdot \psi_j,$$

and the Hessian matrix can be computed by

$$h_{j,k} = \lambda_j \delta_{j,k} - \sum_n f_s(u_i)(\psi_j)_i(\psi_k)_i.$$

If n is small we can take $m = n$ and hence expect nearly exact approximations.

27.3 Algorithms

The notation used in this section is mostly for PDE, but the algorithms immediately apply to PdE. We first outline the mountain pass type algorithms which use steepest descent in Sobolev space. The MPA and MMPA find MI 1 and MI 2 solutions to (27.2), under our standard superlinear hypothesis. Mountain pass type algorithms can be modified to find many types of critical points, but generally require some understanding of the variational structure in order to identify appropriate constraining sets. In [48], higher MI solutions were found by constraining minimizing sequences of functions in S or S_1 to particular invariant fixed point spaces.

We find the more general Newton type algorithms operating in coefficient space to be robust and efficient in solving equations like (27.1) and (27.2). The augmented GNGA below are very good for continuation and branch switching, respectively. Efficiency is enhanced considerably by consideration of symmetry and a carefully chosen basis. In [130, 131] this was done for a particular PDE with fixed symmetry. In [132] we developed a suite of programs which use automatically generated symmetry information to perform continuation and branch switching for PdE on arbitrary graphs. These programs largely achieved our goal to automate the process "from edgelist to solutions." The procedure is fairly complicated and only summarized here. A collection of perl scripts facilitates doing all of the following in an almost complete automatic fashion:

1. Nauty and GAP [74] are used to generate files containing symmetry information for: G, possible solutions to (27.2), and possible bifurcations of branches of solutions to (27.2).
2. Layouts of the graph are automatically generated. There are tools for customizing the choice of layout as well.
3. If not known in closed form, the eigenvectors are obtained via ARPACK for the graph Laplacian L. Among other symmetry related tasks, the basis is indexed to give bases for every fixed point subspace of Γ_0. We use Mathematica for this.
4. Bifurcation digraphs which reveal all possible types of bifurcations are created in machine readable, human readable, and graphical formats.
5. The main C++ program follows a branch from the queue of branches, seeded with an initial trivial solution. Every time a bifurcation point is encountered, new jobs are put on the queue for each non-conjugate solution found on a bifurcating branch. All branches are followed until they exit a window; execution stops when the queue is empty.
6. Gnuplot is used to generate bifurcation diagrams automatically, with several choices of y-coordinate provided. The diagrams are annotated with symmetry and/or MI information, as desired.
7. The Mathematica kernel is used to generate a selection of contour plots of solutions using the chosen graph layout.

At the time of this writing, the above automated branch following code has been slightly modified to be more efficient, particularly in minimizing the amount of computations to form the Hessian. The code is able to accurately approximate solutions to (27.1). For example, with 540 basis vectors and 9261 grid points for $\Omega = (0,1)^3$, after the basis had been generated it took our C++ code about 4 hours on a 3GHZ Linux workstation to find 938 solutions in order to follow branches bifurcating from the first 5 eigenvalues until they exited the window at $s = 0$.

27.3.1 The MPA and MMPA

Consider approximating the MI 1 and MI 2 solutions to (27.1) by minimizing J_s restricted to S and S_1, respectively. Using an $n-$point grid in Ω, we approximate $-\Delta w = f_s(u)$ with a sparse linear system. Solving this system gives us an approximation for the Sobolev gradient $\nabla J_s(u) = u + w$ at the gridpoints. Using

$$P_u \nabla J_s(u) = \frac{J'(u)(u)}{||u||_H^2}\, u,$$

which can be computed using standard numerical integration techniques, the MPA with step-size δ is:

1. let u be a one-sign initial guess
2. Loop until $\nabla J_s(u)$ is small
   a) solve linear system to compute $\nabla J_s(u)$
   b) descent step: $u \leftarrow u - \delta \nabla J_s(u)$
   c) Loop until $u \in S$
      i. ascent step: $u \leftarrow u + \delta P_u \nabla J_s(u)$

The MMPA relies on the fact that $u_+, u_- \in S$ implies that $u{=}u_+{+}u_-{\in}S_1$:

1. let u be a sign-changing initial guess
2. Loop until $\nabla J_s(u)$ is small
   a) solve linear system to compute $\nabla J_s(u)$
   b) descent step: $u \leftarrow u - \delta \nabla J_s(u)$
   c) Loop until $u_+, u_- \in S$ $(u \in S_1)$
      i. ascent step: $u_+ \leftarrow u_+ + \delta P_{u_+} \nabla J_s(u_+)$
      ii. ascent step: $u_- \leftarrow u_- + \delta P_{u_-} \nabla J_s(u_-)$

These algorithms work well, but can only find the specific low MI minimax solutions mentioned. For related problems where f_s is not superlinear, the minimax structure will be different. In many cases, one can identify one or more constraints and use a similar type of ascent/descent step to find select critical points with a particular variational characterization. In [47], for example, sign-changing solutions are found to an asymptotically linear problem using a Lyapunov-Schmidt reduction and steepest ascent/descent in coefficient space.

27.3.2 The GNGA

The GNGA is just Newton's method on the gradient $\nabla J_s(u)$ applied in coefficient space, given the (perhaps carefully chosen) basis $\{\psi_j\}_M$ of eigenfunctions of $-\Delta$ for the finite dimensional subspace A:

1. let a be an initial guess coefficient vector
2. compute $u = \sum_m a_i \psi_i$
3. Loop until $P_A \nabla J_s(u)$ is small
   a) use eigenvalues and numerical integration to compute g and h
   b) solve $h\chi = g$ for the search direction χ
   c) Newton step: $a \leftarrow a - \chi$
   d) compute $u = \sum_m a_i \psi_i$

There are many refinements available in implementing the GNGA. Most importantly, if there is symmetry in the problem then the Hessian matrix h will have a special block structure. By understanding this structure one can have great savings in the costly computation of the entries of h, many of which will be zero. A step-size δ can be used in the Newton step, although if good initial guesses are available this is generally unnecessary and counterproductive. Several standard packages do a good job of solving the linear system for χ each iteration, even when h is singular or nearly so.

The most interesting case where h is singular occurs at bifurcation points, i.e., pairs (u, s) where different branches of solutions intersect in $H \times \mathbb{R}$. In fact, we obtain the necessary good initial guesses by continuation, i.e., starting at a known solutions such as $u = 0$ for some parameter s, and following branches. The tangent GNGA works in $\mathbb{R}^{m+1}$ with an extra constraint; the parameter s is treated as an unknown. Two sequential solutions on a branch are used to follow a tangent of the bifurcation curve and find a next solution on the curve. When two solutions on a branch have a different MI, the secant method applied to one of the eigenvalues of the Hessian h is employed to find a degenerate point in between. We in fact use a sort of bisection and apply a secant method on recursively divided subintervals until all degenerate points between the original two points have been found. After analyzing a degenerate point and identifying it as a bifurcation point (as opposed to a fold point), bifurcation theory is used to obtain new solutions on different, bifurcating branches. In particular, if (u_*, s_*) is a bifurcation point, then vectors e in the critical eigenspace E are generally candidate perturbations for solutions, i.e., $(u_* + \delta e, s_*)$ can be used as an initial guess for a solution on a new branch. Here again symmetry can be used to great effect; if E is not one dimensional it can often be decomposed into subspaces guaranteed to lead to new solutions with particular symmetries. If one is searching within a component of E of large dimension, then a large number of random guesses within that component may be necessary in order to find most if not all bifurcating branches. The cylinder GNGA works in $\mathbb{R}^{m+1}$ with a different extra constraint which generally ensures that new solutions lie off of the parent branch, perturbed by a particular component of E.

27.3.3 Tangent-Augmented Newton's Method (tGNGA)

Given two consecutive solutions p_o and p_c on a given branch, we compute the normalized tangent vector

$$v = (p_c - p_o)/||p_c - p_o|| \in \mathbb{R}^{m+1}.$$

The initial guess is then $p_g = p_c + cv$. In our experiments the speed c has a minimum and maximum range, and is modified dynamically according to various heuristics (see for example Figure 27.4). For the tGNGA, the constraint is that each iterate $p = (a, s)$ must lie on the hyperplane passing through the initial guess p_g, perpendicular to v. That is, $\kappa(a, s) := (p - p_g) \cdot v$. Easily, one sees that $(\nabla_a \kappa(a, s), \frac{\partial \kappa}{\partial s}(a, s)) = v$ and that $g_s(a) = (a_j(\lambda_j - s) - (\text{nonlinearterm}))_{j=1}^m$ implies $\frac{\partial g}{\partial s} = -a$. Newton's method is invariant in this plane so that in fact $\chi \cdot v = 0$ at each step. Hence, the linear system to be solved each iteration can be described by:

$$\begin{bmatrix} h & -a \\ (v_a)^T & v_s \end{bmatrix} \begin{bmatrix} \chi_a \\ \chi_s \end{bmatrix} = \begin{bmatrix} g \\ 0 \end{bmatrix},$$

where for appearance $v = (v_a, v_s) \in \mathbb{R}^{m+1}$ can be partitioned into 2 components. Our function `tGNGA(`p_g`,` v`)` returns, if successful, a new solution p_n to (27.1) or (27.2), satisfying the tangent constraint constraint.

27.3.4 The Secant Method

In brief, when using the tGNGA to follow a solution branch and the MI changes at consecutively found solutions, say from k at the solution p_o to $k + d$ at the solution p_c, we know by the continuity of $D^2 J_s$ that there exists a third, nearby solution p^* where h is not invertible and the r^{th} eigenvalue of h is zero, where $r = k + \lceil \frac{d}{2} \rceil$. We effectively employ the vector secant method to find a degenerate point on this segment of bifurcation curve.

Let $p_0 = p_o$, $p_1 = p_c$, with β_0 and β_1 the r^{th} eigenvalues of h at the points p_0 and p_1, respectively. Then iterate:

- $p_g = p_i - \dfrac{(p_i - p_{i-1})\beta_i}{(\beta_i - \beta_{i-1})}$
- $p_{i+1} = \mathtt{tGNGA}(p_g, v)$

until the sequence (p_i) converges. The vector $v = (p_c - p_o)/||p_c - p_o||$ is held fixed throughout, while the value β_i is the newly computed r^{th} eigenvalue of h at p_i. Our function `secant(`p_o`, `p_c`)` returns, if successful, a solution point $p^* = (a^*, s^*)$ lying between p_o and p_c where h is not invertible. Hence, p^* will be a candidate bifurcation point.

27.3.5 Cylinder-Augmented Newton's Method (cGNGA)

The cGNGA is used to find initial solution points on new branches near bifurcation points p^* where h is not invertible and hence $he = 0$ has a nontrivial subspace of solutions $e \in \mathbb{R}^m$. After such a point has been detected the corresponding critical eigenspace E is computed via a call to an LAPACK eigenvalue solver. If the dimension of E is large, many random guesses will be required in order to have confidence that most if not all bifurcating solutions have been found. We in fact decompose E into the possible symmetry invariant subspaces $\{E_k\}$ of that critical eigenspace, as dictated by the automatically generated bifurcation digraph (see [131] for more on this generalization of the well known lattice of isotropy subgroups). These spaces are typically low-dimensional and do not require many different random guesses to be made.

With E (or some E_k) in hand, we search for a new solution off of a parent branch by enforcing the condition

$$\kappa(a, s) = \frac{1}{2}(|P_E a|^2 - \epsilon^2) = 0.$$

The radius ϵ is a small fixed parameter. That is, we insist that the Newton iterates belong to the cylinder $C = \{p \in \mathbb{R}^{n+1} : |P_E a| = \epsilon\}$. The initial guess $p_g := p^* + \epsilon(e, 0)$, where e is any randomly chosen unit vector in E, lies on the cylinder C. Typically, solutions on the parent branch satisfy $|P_E a| = 0$ in which case the new solution belongs to a child branch of lesser symmetry. Easily one sees that

$$\nabla_a \kappa(a, s) = (P_E)^T P_E a = P_E a, \; \frac{\partial \kappa}{\partial s}(a, s) = 0,$$

and again $\frac{\partial g}{\partial s} = -a$. Hence, the search direction χ is found by solving

$$\begin{bmatrix} h & -a \\ (P_E a)^T & 0 \end{bmatrix} \begin{bmatrix} \chi_a \\ \chi_s \end{bmatrix} = \begin{bmatrix} g \\ \kappa \end{bmatrix}.$$

When successful, cGNGA(p^*, p_g, E) returns a new solution p_n of (27.1) or (27.2) that lies on the cylinder C.

27.4 Some PDE and PdE Results

Mathematica or Matlab programs to solve (27.1) in the ODE case via mountain pass and GNGA algorithms can be coded in just a few lines. Depending on boundary conditions, sines and/or cosines can be used to populate a relatively small matrix with a basis for the discretized problem. For the types of equations currently under our consideration, all solutions that we find via mountain pass type algorithms can equally well be found via our Newton code.

Our first GNGA code was applied in [129] to the case $\Omega = (0,1)^2$. Much manual trial and error was used to effect branch switching and continuation. Symmetry was observed and analyzed but not fully used, certainly not in any automated way. In [130,131] we consider the case where Ω is a region with d_6 symmetry bounded by Koch's snowflake. Here the symmetry was analyzed by hand and used to write code that automated the branch following. Figure 27.4 contains a bifurcation diagram from that experiment. Included is a branch of MI 2 minimal energy sign-changing exactly-once solutions from [34]. The MMPA could also find these CCN solutions, one of which is depicted in Figure 27.4.

When applying the augmented GNGA to PdE, it was natural to embrace symmetry. One type of experiment involved picking a desired symmetry group first, then building a graph that had that symmetry. In Figure 27.4, we see the first primary branch and all of its secondary branches for the Cayley graph. This graph has 9 vertices and 12 edges and is a level one pre-fractal graph for the Sierpinski gasket . The bifurcation points on the primary branch can be shown to occur at $s = -\lambda_i/2$ for this nonlinearity. In this diagram each solution on the interpolating curve is marked with a plus, thus showing the effect of our heuristics for adjusting the branch following speed. When a branch has a large curvature or many bifurcation points in a small area, for example, the speed is automatically decreased, while in the absence of interesting behavior, the speed is increased.

A bifurcation digraph annotated with contour plots explaining the symmetry of solutions to (27.4) S_3 can be found in Figure 27.4. The possible types of bifurcations are the arrows between symmetry types. This information is used to reduce the dimension of search spaces when using the cGNGA to find bifurcating solutions.

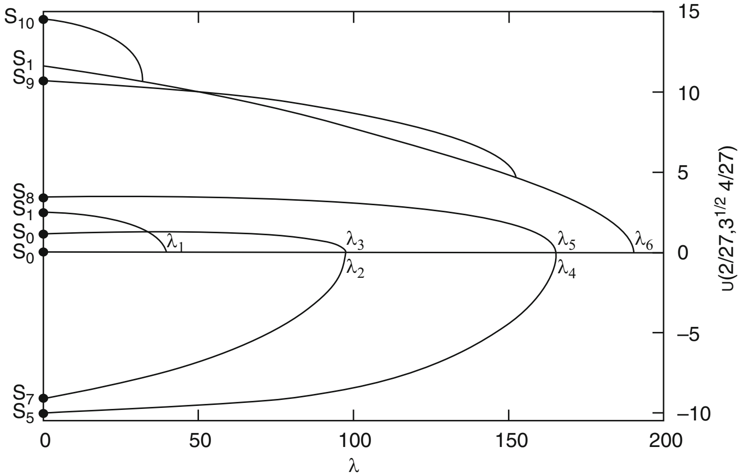

Fig. 27.1 The complete bifurcation diagram for the first six primary branches bifurcating from the trivial branch for (27.4). Here, Ω is a region bounded by Koch's snowflake and the $y-axis$ of the plot is the u value of the solution evaluated at a generic point of the grid. The dot at $\lambda = 0$ with symmetry S_7 is a CCN solution and is depicted in Figure 27.4 along with a solution with symmetry S_{10}. We used the level 5 grid of equilateral triangles with 11,605 vertices and 300 modes in approximating these solutions.

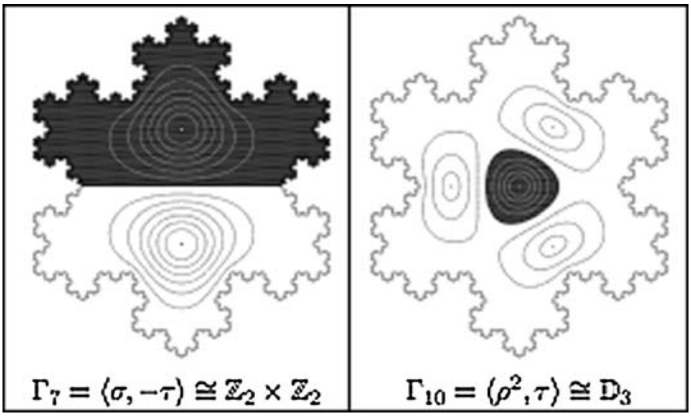

Fig. 27.2 Contour plots of solutions with symmetry types S_7 and S_{10} at $\lambda = 0$. Solutions of all 23 possible symmetries were found. The CCN solution on the left is even in x and odd in y, while the higher MI solution on the right is even in y and invariant under rotations by $2\pi/3$.

Although the MPA and MMPA require knowledge of variational structure and can be hard to apply for different nonlinearities f_s, the augmented GNGA work well for a variety of different equations. Figure 27.4 shows the bifurcation

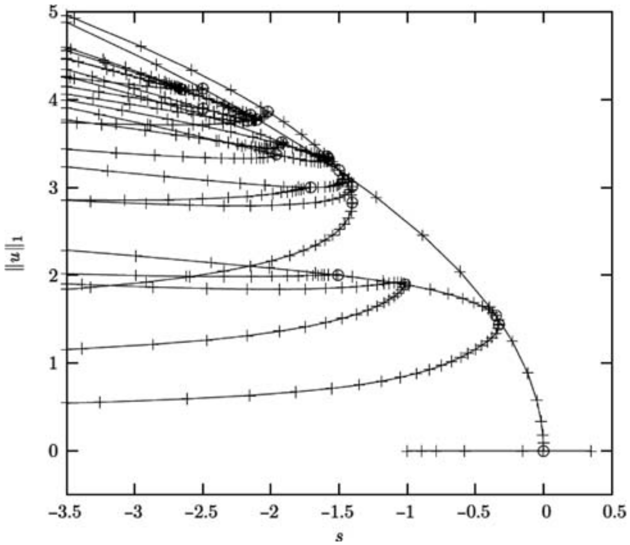

Fig. 27.3 Bifurcation diagram for the first primary branch and its secondary branches for the Cayley graph of S_3. The graphic demonstrates how the density of points is increased near interesting features. We use heuristics to adjust the speed. For example, the speed c is halved if tGNGA fails to converge in four iterations. Further, the speed is multiplied by a factor in $(0, 2]$ based on the angle formed by the last three points, where the factor is 1 if the angle is 0.1 radians.

Fig. 27.4 Bifurcation diagram for a non-odd, non-superlinear f_s on P_3, the path with 3 vertices.

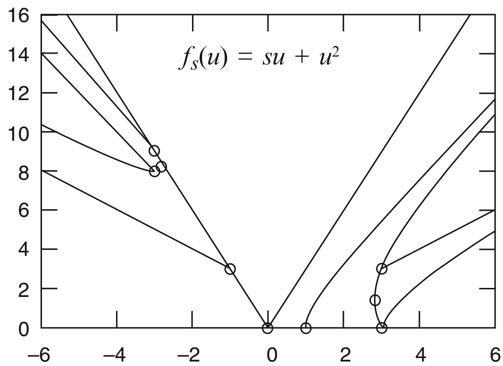

diagram for the path with 3 vertices and a non-odd, non-superlinear problem. There is no difficulty in following branches to the right as well as left.

As a final example, the CCN solution and two higher MI solutions on the truncated icosahedron are displayed in Figure 27.4. It will be interesting to increase the number of vertices and consider a graph approximating the surface of a sphere.

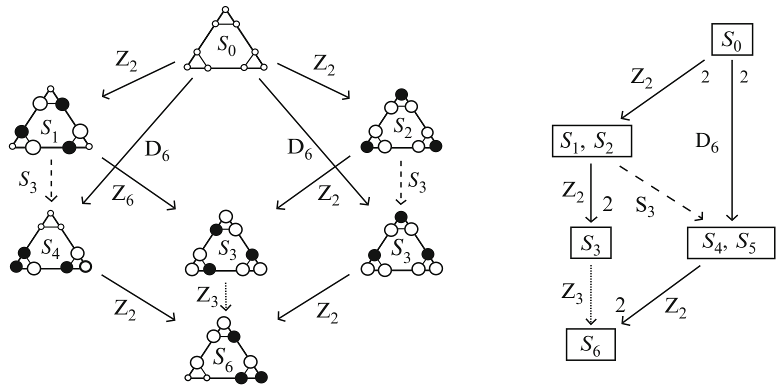

Fig. 27.5 Bifurcation digraphs for a decorated Cayley graph of S_3. The digraph on the left is not condensed while the digraph on the right is condensed. The embedded contour plots were automatically generated from numerical solutions to (27.2).

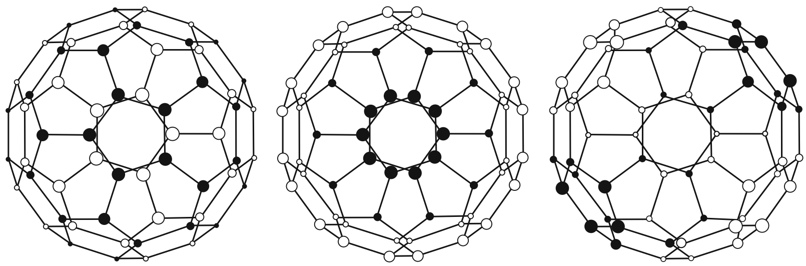

Fig. 27.6 Contour plots of three solutions to 27.2 for the truncated icosahedron. The MI 2 CCN solution (left) has 20 symmetries, all visible in this layout. The front hemisphere is positive and the back is negative. The MI 5 solution (center) has 20 of 20 visible symmetries as well. It has a negative equatorial band separating front and back positive caps. The MI 6 solution (right) has 8 symmetries of which only 4 are visible. The nodal structure with two positive and two negative components is clear. All three solutions are very close to eigenvectors of L, which in turn resemble eigenfunctions of the PDE Laplacian $-\Delta$ on the sphere. Specifically, they have similar nodal structures as the spherical harmonics $Y_{1,0}$, $Y_{2,0}$, and $\mathrm{Re}\,(Y_{2,2})$.

Chapter 28
Ginzburg-Landau Separation Problems

S. Sial

28.1 Introduction

Many problems in mathematical physics can be formulated in terms of finding the minima of energy functionals. These minimum energy states are interpreted as stable (or perhaps metastable) equilibria of the physical systems that the energy functionals are supposed to characterize. We are interested in prototypical models used for studying pattern formation or ordering, such as nucleation and spinodal decomposition.

The Sobolev gradient approach has proven to be very succesful in finding the minimum energy states for various Ginzburg-Landau functionals of physical interest [185, 212–214] as well as Chapters 13 ,14.

If $F(u)$ is a Ginzburg-Landau functional, then the overdamped Ginzburg-Landau time evolution of the order parameter u is given by

$$u_t \;=\; -\nabla F(u) \tag{28.1}$$

Note that this is continuous steepest descent, the gradient $\nabla F(u)$ points in the direction of greatest increase of the functional F and $-\nabla F(u)$ takes the system in the direction that decreases the functional F the fastest.

Even if one were not interested in the time evolution itself, this suggests a means to numerically investigate the minimum energy states. Substituting a Sobolev gradient for the gradient in 28.1 leads to a much smoother approach to the equilibrium state.

This chapter will discuss models A and B in the Halperin-Hohenberg taxonomy, [82] in which the coarse-grained field or the order parameter is either not conserved (model A) or conserved (model B) as well as a new model A' as an alternative to model B, [213].

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_28,

28.2 Model A

In a Ginzburg-Landau type model one seeks to capture the essential features of a system without going into all of the details. This is done by constructing a free energy functional whose argument is an order parameter (perhaps more than one) that characterizes the system. The symmetries and main features of the of the physical system are built into the model free energy functional.

Suppose that we have a system characterized by an order parameter that takes on equilibrium values $+1$ or -1 with equal likelihood when there are no values fixed at the boundaries. This could be modelled by a free energy functional whose integrand is an energy density given by a polynomial of even powers in the order parameter u. That way, the substitution of $-u$ for u produces no change in the total free energy. Suppose that we also know that the system as it evolves develops regions of positive and negative u. Then we can impose an energy penalty for gradients in the free energy functional.

A model A functional might have a form like

$$F(u) \;=\; \int_{\Omega} \frac{1}{4}u^4 \;-\; \frac{1}{2}u^2 \;+\; \frac{\kappa}{2}|\nabla u|^2 \tag{28.2}$$

The parameter κ will determine the width of interfaces between regions of positive and negative u. The problem of minimization then can also be thought of as a problem in determining interfaces.

For numerical minimization, consider a uniform grid. One possible finite-dimensional analogue of 28.2 would be

$$F(u) \;=\; < D_0(u^4/4 - u^2/2), 1 > + \sum_i \kappa < D_i(u), D_i(u) >$$

where the D_i are finite difference estimates of derivatives as given elsewhere in this volume and $<,>$ is the Euclidean inner product.

We can now calculate the gradient of the functional, and then move the system in the opposite direction in function space in order to minimize the energy using steepest descent. The gradient $P\nabla F$ is calculated by solving

$$\pi(D_0^t D_0 + \sum_i D_i^t D_i)P\nabla F(u) = \pi\nabla F(u)$$

where π is the projection that sets vectors to zero on the boundaries, $\nabla F(u)$ is the gradient calculated with respect to the Euclidean inner product and P is the orthogonal projection onto the range of D (see Chapter 10). Steepest descent then minimizes the energy by repeated steps

$$u \to u - \lambda P\nabla F(u)$$

where λ is a fixed positive constant.

28.3 Weighted Gradients

The parameter κ that has not been considered up until now. Motivated by an approach previously developed for singular ODEs and PDEs, ([118] and Section 29.1 of Chapter 30) one can define a new Sobolev space $H_1^2(\kappa)$ equipped with an inner product

$$(u, v) \;=\; < u, v > \;+\; \kappa < D_1 u, D_1 v >$$

which now takes κ into account. Some preliminary results in other applications of Sobolev gradients suggests that a weighted gradient is particularly helpful in cases where a parameter varies sharply across the grid.

28.4 Model A′

For model A type systems, the order parameter u is not conserved. Model B or a Cahn-Hilliard [82] system has a dynamics given by

$$u_t \;=\; \Gamma \nabla^2 \left(\nabla F(u) \right)$$

where Γ is a constant and F is a model A functional. Here the integral of u remains constant and it is said that u is conserved. Numerically, the problem will require fourth order operators.

If however, one is not interested in the dynamics which leads to a critical point but rather in the equilibrium states reached under this conservation constraint, there is another model possible which has been called model A′ [213] The idea of model A′ is to minimize a model A functional subject to the constraint of conservation.

Previously, the numerical scheme required a projection P from L_2 to H_1^2. To preserve the integral of u one needs a projection Q onto the space of functions with integral zero. The L_2 gradient has to be repeatedly acted on by P and Q until convergence. Numerically, this can be done within a conjugate gradient or other solver so that a conjugate gradient step alternates with a projection onto the space of functions with integral zero. We see that minimization in model A′ can be done as easily as in model A.

In the next two sections there are two more applications of Sobolev gradient methods, one to a phase separation problem and another to a problem in elasticity.

28.5 A Phase Separation Problem

A typical result of this model of phase separation is shown in Figure 28.1. In this example, on a square disk $\Omega = [0,1]^2$, with $\alpha = 2., T = .8$, consider the energy functional F so that

$$F(u) = \int_{\Omega} \frac{\alpha}{4} - \frac{T}{2}(1+u)\ln\frac{1+u}{2} + \frac{T}{2}(1-u)\ln\frac{1-u}{2} + \frac{\kappa}{2}\|\nabla u\|^2, \; u \in H^{1,2}(\Omega). \tag{28.3}$$

Boundary conditions are as follows: On the lower edge, $u = .5$, on the upper and left edges $u = 0$, and on the right edge, $u = -.5$. Figure 28.1 shows clear separation of the two substances for the order parameter u of (28.3).

The convergence properties of the method are also worth noting. The grids were strictly uniform. Interfaces were not treated specially and neither was much effort made to start with a good guess for the final configuration. Still, convergence was not a problem. Thus the method is suitable for situations in which one wishes to have an algorithm for interface problems that will converge without any intervention.

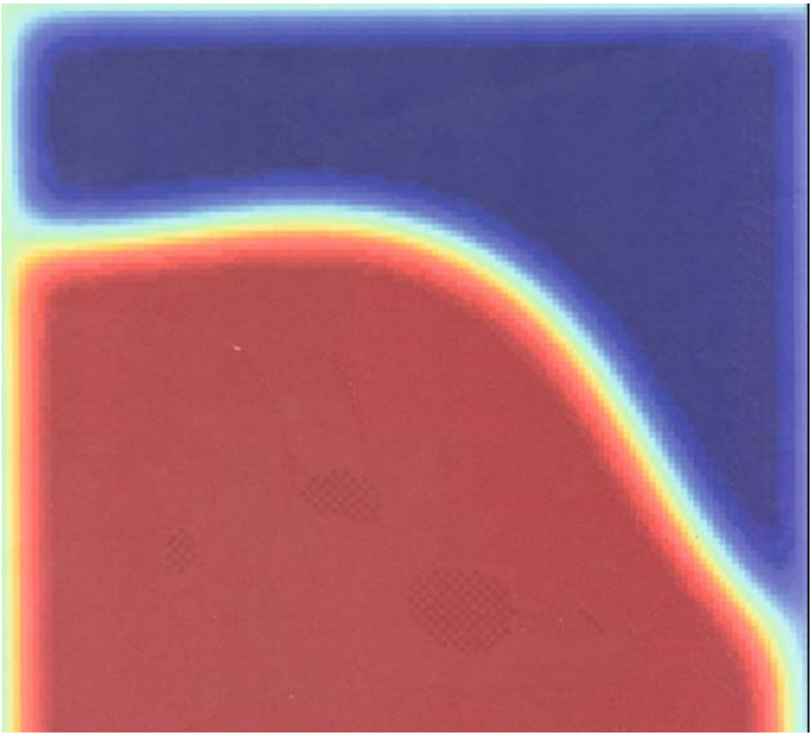

Fig. 28.1 Oil-water Separation Example

28.6 An Elasticity Problem

The following problem in elasticity was similarly treated. It resulted from collaboration with J. Neuberger, T. Lookman and A. Saxena.

On a square region $\Omega \subset R^2$ and $(u, v) \in H = H^{1,2}(\Omega)^2$, define

$$\phi(u, v) = \int_\Omega (E(u, v)^4 - E(u, v)^2 + \|(\nabla E)(u, v)\|^2 + \frac{1}{2}F(u, v)^2 + G(u, v)^2)$$

where

$$\begin{aligned} 2 * E(u, v) &= u_1 + v_2 \ (deviatoric) \\ 2 * F(u, v) &= u_1 - v_2 \ (compression) \\ 2 * G(u, v) &= u_2 + v_1 \ (shear) \end{aligned}$$

Conditions on the boundary are $v = 0$ on $\partial\Omega$, $u = 0$, bottom and left, u linear on the top and right of $\partial\Omega$. A resulting graph of displacement, Figure 28.2, follows.

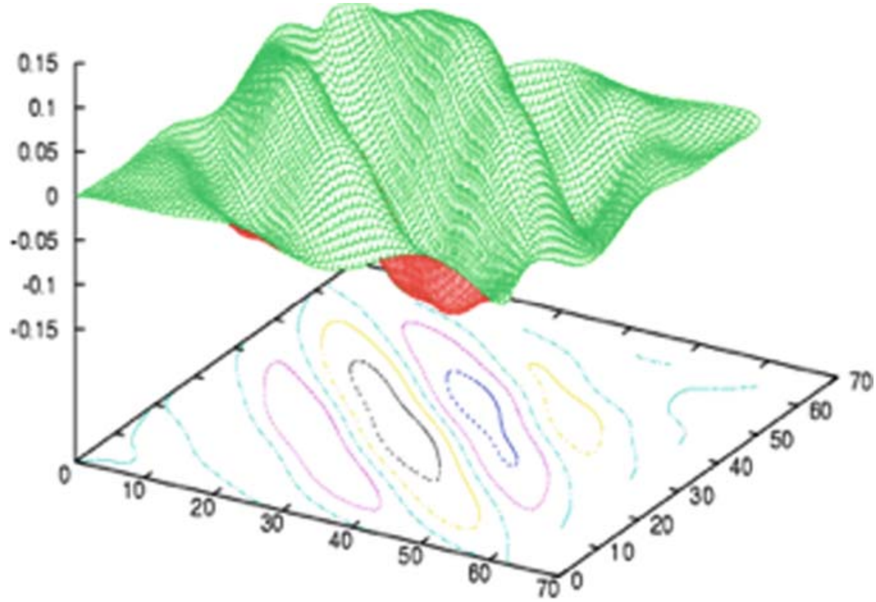

Fig. 28.2 Displacement Due to Stress

Chapter 29
Numerical Preconditioning Methods for Elliptic PDEs

J. Karatson

29.1 Introduction

Solution methods for nonlinear boundary value problems form one of the most important topics in applied mathematics and, similarly to linear equations, preconditioned iterative methods are the most efficient tools to solve such problems. For linear equations, the theory of equivalent operators in Hilbert space has proved an efficient framework for the study of preconditioners, developed in [60, 72, 119], see also the summary [9]. Hereby one uses the discretization of a suitable linear elliptic operator as preconditioning matrix, and as a result, one in particular obtains mesh independent convergence rates. In the present paper we propose that the Sobolev gradient approach, coupled with the preconditioning operator idea, is a nonlinear analogue of the equivalent operator idea that provides an efficient organized framework of iterative methods for nonlinear elliptic problems.

In the Sobolev gradient approach the iteration is constructed as a gradient (steepest descent) method for a suitable functional. The main principle of Sobolev gradients is that preconditioning can be obtained via a change of inner product to determine the gradient of the functional. In particular, a sometimes dramatic improvement can be achieved by using the Sobolev inner product instead of the original L^2 one. See the demonstrative example in Chapter 2, and for further discussion in preceding chapters. (Related ideas are used in the so-called H^1-methods, see e.g. in [200, 201]. The change of inner product appears in the iterative sequence as a preconditioning operator (or rather its discrete version when the algebraic system arising from FEM or FDM discretization of the PDE is solved). The scope of Sobolev gradients includes least-square functionals for general operators, but in this paper we consider elliptic potential operators and minimize the corresponding potential as in Chapter 11. In this context the above-mentioned operator in the iterative sequence leads to the concept of preconditioning operators from the monograph [61]. This preconditioning operator is the minus Laplacian or $Su \equiv -\Delta u + cu$ when the standard Sobolev inner product is used, and, more generally, a suitable general elliptic operator when a weighted Sobolev

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inner product is applied (see e.g. [115–117]). Here a general iterative solution method for a nonlinear elliptic BVP $F(u) = b$ is given by the projection of a sequence

$$u_{n+1} = u_n - B_n^{-1}(F(u_n) - b)$$

into the discretization subspace, where B_n are suitable linear elliptic operators, either fixed ($B_n \equiv B$) or stepwise variable. Altogether, the concepts of Sobolev gradients and preconditioning operators can be here understood on a common basis.

Based on the above, our goal is to present that the Sobolev gradient idea is able to provide a general framework to discuss iterative methods via the concept of preconditioning, and the scope of this framework reaches from simple iterations to Newton methods.

We present these ideas on a simple model Dirichlet problem; more general problems are referred to at the end. First, our discussion starts with fixed preconditioners. We begin with an exposition of the Sobolev gradient idea with the standard H_0^1 inner product, leading to Laplacian preconditioners, then fixed weighted inner products are used to derive general linear elliptic preconditioners. Second, we allow the stepwise change of the inner product and obtain variable preconditioners (including the case of Newton-like iterations) as gradients w.r. to a variable inner product in the Sobolev space. In particular, Newton's method can be regarded as an optimal extreme case of variable steepest descent.

Throughout the whole paper, we identify any occurring Hilbert space H with its dual H', based on the Riesz representation theorem. That is, if a bounded linear functional $\phi \in H'$ satisfies $\phi v = \langle b, v \rangle$ with $b \in H$, then we identify ϕ with b. In particular, mappings from H to $\mathbf{R}$ will have gradients in H.

29.2 The Model Problem

For ease of presentation we consider the Dirichlet problem

$$\begin{cases} T(u) \equiv -\mathrm{div}\, f(x, \nabla u) = g(x) \\ u_{|\partial\Omega} = 0 \end{cases} \tag{29.1}$$

with standard smoothness and ellipticity assumptions:

Assumptions 29.2.1.

(i) The function $f : \Omega \times \mathbf{R}^N \to \mathbf{R}^N$ is measurable and bounded w.r. to the variable $x \in \Omega$ and C^1 w.r. to the variable $\eta \in \mathbf{R}^N$, further, its Jacobians $\frac{\partial f(x,\eta)}{\partial \eta}$ are symmetric and satisfy

$$\mu_1 G(x)\xi\cdot\xi \le \frac{\partial f(x,\eta)}{\partial\eta}\xi\cdot\xi \le \mu_2 G(x)\xi\cdot\xi \qquad ((x,\eta)\in\Omega\times\mathbf{R}^N,\ \xi\in\mathbf{R}^N)$$

with constants $\mu_2 \ge \mu_1 > 0$ independent of (x,η).

(ii) $g \in L^2(\Omega)$.

More general problems will be referred to in section 29.6.

In what follows, $H_0^1(\Omega)$ is the real Sobolev space with the inner product

$$\langle u,v\rangle_{H_0^1} := \int_\Omega \nabla u\cdot\nabla v. \tag{29.2}$$

The above assumptions ensure that problem (29.1) has a unique weak solution $u^* \in H_0^1(\Omega)$.

Letting $V_h \subset H_0^1(\Omega)$ be a finite element subspace of the real Sobolev space $H_0^1(\Omega)$, we wish to find the unique FEM solution of (29.1) in V_h.

29.3 Condition Numbers of Nonlinear Operators

The following notion (see e.g. [61, 92]) will be required in the next section.

Definition 29.1. Let H be a real Hilbert space and let A be a strictly monotone nonlinear operator in H. Then the *condition number* of A is defined as

$$cond(A) = \frac{\Lambda(A)}{l(A)},$$

where

$$\Lambda(A) = \sup_{u\neq v\in D(A)} \frac{\langle A(v)-A(u), v-u\rangle}{\|v-u\|^2}$$

$$\lambda(A) = \inf_{u\neq v\in D(A)} \frac{\langle A(v)-A(u), v-u\rangle}{\|v-u\|^2}.$$

The numbers $\Lambda(A)$ and $\lambda(A)$ are called the *spectral bounds of A*. Similarly to the linear case, there holds $0 < \Lambda(A) \le \infty$, $0 \le l(A) < \infty$. We emphasize that the condition number may be infinite, as is the case for the differential operator in (29.1). Namely, there holds

$$\begin{aligned}\langle T(v)-T(u), v-u\rangle &= \int_\Omega (f(x,\nabla v)-f(x,\nabla u))\cdot(\nabla v-\nabla u)\\ &= \int_\Omega \frac{\partial f}{\partial\eta}(x,\nabla u+\theta\nabla(v-u))\,(\nabla v-\nabla u)\cdot(\nabla v-\nabla u)\\ &\ge \mu_1\int_\Omega |\nabla(v-u)|^2,\end{aligned}$$

hence

$$\Lambda(T) \geq \mu_1 \sup_{u \neq v \in D(T)} \frac{\int_\Omega |\nabla(v-u)|^2}{\int_\Omega |v-u|^2} = \mu_1 \sup_{z \neq 0 \in D(T)} \frac{\int_\Omega |\nabla z|^2}{\int_\Omega |z|^2} = \infty\,,$$

that is,

$$cond(T) = \infty. \tag{29.3}$$

29.4 Fixed Preconditioners: Sobolev Gradients with Fixed Inner Product

Assumptions 29.2.1 on f imply the existence of a function $\psi : \Omega \times \mathbf{R}^N \to \mathbf{R}$ with

$$\frac{\partial \psi}{\partial \eta}(x, \eta) = f(x, \eta),$$

hence we can introduce the functional $\phi : H_0^1(\Omega) \to \mathbf{R}$,

$$\phi(u) \equiv \int_\Omega \psi(x, \nabla u)\,. \tag{29.4}$$

Then, by a simple calculation, the directional derivatives of ϕ satisfy

$$\frac{\partial \phi}{\partial v}(u) = \int_\Omega f(x, \nabla u) \cdot \nabla v \qquad (u, v \in H_0^1(\Omega)). \tag{29.5}$$

Using the divergence theorem, we can write (29.5) as

$$\frac{\partial \phi}{\partial v}(u) = \int_\Omega T(u) v \qquad (u, v \in H^2(\Omega) \cap H_0^1(\Omega)). \tag{29.6}$$

Since for fixed u the linear functional $v \mapsto \int_\Omega T(u)v$ is bounded in $L^2(\Omega)$, we obtain by definition that ϕ is Gateaux differentiable as a functional from $L^2(\Omega)$ to $\mathbf{R}$ (with the dense domain $D(\phi) = D(T) = H^2(\Omega) \cap H_0^1(\Omega)$). Further, (29.6) gives that the L^2-gradient is

$$\phi'(u) = T(u) \qquad (u \in H^2(\Omega) \cap H_0^1(\Omega)). \tag{29.7}$$

The L^2-gradient (29.7) will now be replaced by Sobolev gradients in two steps. First, we start with explaining the Sobolev gradient idea with the usual H_0^1 inner product, which leads to Laplacian preconditioners. Then more general preconditioners will be discussed as Sobolev gradients w.r.t. to a fixed weighted inner product in $H_0^1(\Omega)$.

29.4.1 Sobolev Gradients and Laplacian Preconditioners

Let the space $H_0^1(\Omega)$ be endowed with the usual inner product

$$\langle u, v \rangle_{H_0^1} = \int_\Omega \nabla u \cdot \nabla v \tag{29.8}$$

and let us consider the generalized differential operator

$$F : H_0^1(\Omega) \to H_0^1(\Omega)$$

corresponding to (29.1), i.e.

$$\langle F(u), v \rangle_{H_0^1} = \int_\Omega f(x, \nabla u) \cdot \nabla v \qquad (u, v \in H_0^1(\Omega)), \tag{29.9}$$

where for any fixed $u \in H_0^1(\Omega)$ the existence of $F(u) \in H_0^1(\Omega)$ is ensured by the boundedness of the r.h.s. as a functional $H_0^1(\Omega) \to \mathbf{R}$ in v and by our convention to identify any Hilbert space with its dual.

Then, using the preceding arguments, ϕ is Gateaux differentiable as a functional from $H_0^1(\Omega)$ to $\mathbf{R}$, and by (29.5) and (29.9) the H_0^1-gradient is

$$\phi'_{H_0^1}(u) = F(u) \qquad (u \in H_0^1(\Omega)). \tag{29.10}$$

In particular, the operator

$$-\Delta \text{ on } H^2(\Omega) \cap H_0^1(\Omega)$$

maps onto $L^2(\Omega)$ under the regularity assumption that Ω is C^2-diffeomorphic to a convex domain [89], hence in this case we have the decomposition

$$F_{|H^2 \cap H_0^1} = (-\Delta)^{-1} T \tag{29.11}$$

and (29.10) can be replaced by

$$\phi'_{H_0^1}(u) = (-\Delta)^{-1} T(u) \qquad (u \in H^2(\Omega) \cap H_0^1(\Omega)). \tag{29.12}$$

That is, the modified gradient (29.10) is expressed as the formally preconditioned version of the original one (29.7) by the operator $-\Delta$.

The steepest descent iteration corresponding to the gradient (29.10) (and with optimal constant stepsize) in V_h is the preconditioned sequence $(u_n) \subset V_h$ defined by

$$u_{n+1} = u_n - \tfrac{2}{M+m} z_n \,,$$
$$\text{where } \langle z_n, v\rangle_{H_0^1} = \langle F(u_n), v\rangle_{H_0^1} - \langle g, v\rangle \quad (\forall v \in V_h),$$

i.e. z_n is the FEM solution of the auxiliary linear Poisson problem

$$-\varDelta z_n = T(u_n) - g, z_{n|\partial\varOmega} = 0$$

in the subspace V_h. It is well-known that u_n converges linearly to the FEM solution in V_h, see e.g. [69] or in the present setting [61, Th. 7.1]. Using the notations of the latter, we obtain

$$cond(F) = cond(-\varDelta^{-1}T) \le \frac{\mu_2}{\mu_1} \tag{29.13}$$

and the corresponding convergence factor

$$q = \frac{\mu_2 - \mu_1}{\mu_2 + \mu_1}\,, \tag{29.14}$$

where $\mu_2 \ge \mu_1 > 0$ are the spectral bounds of the Jacobians of f in assumptions 29.2.1. Note that q is mesh independent, i.e. independent of the subspace V_h.

On the contrary, the steepest descent iteration corresponding to (29.7) would give no convergence, since $cond(T) = \infty$ by (29.3).

The above considerations mean that Sobolev gradient idea, i.e. the transition from L^2-gradient (29.7) to the H_0^1-gradient (29.10), gives a fundamental improvement in the convergence of the corresponding steepest descent iteration. This is an analogue of the phenomenon described in the demonstrative example in Chapter 2.

Remark 29.2. There exist at least three distinct approaches in literature that lead to (discrete) Laplacian preconditioners. Naturally, all their ideas have appeared, at least implicitly, in the above considerations. Let us list them here:

(i) In [198] as well as throughout the present volume the minus Laplacian is frequently the generator of the energy space $H_0^1(\varOmega)$ in which the gradient of the potential ϕ is bounded, in contrast to the L^2-gradient. The construction of the H_0^1-gradient leads to the preconditioner $-\varDelta$. (If the H^1-inner product is used on $H_0^1(\varOmega)$ then the preconditioner becomes $Su = -\varDelta u + u$.)

(ii) In [69,103] the generalized differential operator F in (29.9) is bounded and differentiable in $H_0^1(\varOmega)$, and it has a finite condition number in contrast to T. Hence the simple iteration for F converges linearly in H_0^1-norm. The constructive form of this iteration involves the decomposition (29.11) and hence contains the Laplacian preconditioner.

(iii) In order to achieve a finite condition [10] number, we can naturally compensate for the unboundedness of the nonlinear operator T with a linear elliptic preconditioning operator in similar divergence form. The Laplacian is the simplest operator of this type. In the discrete case, for scalar nonlinearity, T_h and $-\Delta_h$ have the decomposed matrix forms $B^t M(u_h) B$ and $B^t B$, respectively, where B^t denotes the transpose of B.

These ideas reflect different realizations of a common feature, and all of them are captured by the Sobolev gradient idea.

29.4.2 General Preconditioners as Weighted Sobolev Gradients

Let us now endow the space $H_0^1(\Omega)$ with the weighted inner product

$$\langle u, v\rangle_G := \int_\Omega G(x)\, \nabla u \cdot \nabla v\,, \tag{29.15}$$

where the symmetric matrix-valued function $G \in L^\infty(\Omega, \mathbf{R}^{N\times N})$ is spectrally equivalent to the Jacobians of f, i.e. there exist constants $M \geq m > 0$ such that

$$m\, G(x)\xi \cdot \xi \leq \frac{\partial f(x,\eta)}{\partial \eta}\, \xi \cdot \xi \leq M\, G(x)\xi \cdot \xi \qquad ((x,\eta) \in \Omega \times \mathbf{R}^N,\ \xi \in \mathbf{R}^N). \tag{29.16}$$

The inner product $\langle ., .\rangle_G$ is equivalent to the usual one (29.8).

Let us consider the generalized differential operator $F_G : H_0^1(\Omega) \to H_0^1(\Omega)$ under the inner product (29.15), i.e.

$$\langle F_G(u), v\rangle_G = \int_\Omega f(x, \nabla u) \cdot \nabla v \qquad (u, v \in H_0^1(\Omega)). \tag{29.17}$$

The existence of F_G is seen similarly to F in (29.9), we note that here F_G depends on the choice of G. Then, similarly as above, the functional ϕ : $H_0^1(\Omega) \to \mathbf{R}$ in (29.4) is Gateaux differentiable, and the H_0^1-gradient w.r. to the inner product $\langle ., .\rangle_G$ is

$$\phi'_G(u) = F_G(u) \qquad (u \in H_0^1(\Omega)). \tag{29.18}$$

Now the space $H_0^1(\Omega)$ with the inner product (29.15) is the energy space of the operator

$$Su \equiv -\mathrm{div}\,(G(x)\nabla u), \tag{29.19}$$

and under the regularity assumptions $G \in C^1(\overline{\Omega}, \mathbf{R}^{N\times N})$ and that Ω is C^2-diffeomorphic to a convex domain, we have the decomposition

$$(F_G)_{|H^2 \cap H_0^1} = S^{-1} T$$

analogously to (29.11). Hence (29.18) can be replaced by

$$\phi'_G(u) = S^{-1}T(u) \qquad (u \in D(S)). \tag{29.20}$$

That is, the modified H_0^1-gradient (29.18) is expressed as the formally preconditioned version of the original L^2-gradient (29.7) by the operator S.

The steepest descent iteration corresponding to the gradient (29.18) (and with optimal constant stepsize) in V_h is the preconditioned sequence $(u_n) \subset V_h$ defined by

$$u_{n+1} = u_n - \tfrac{2}{M+m} z_n\,,$$
$$\text{where } \langle z_n, v\rangle_G = \langle F_G(u_n), v\rangle_G - \langle g, v\rangle \quad (\forall v \in V_h),$$

i.e. z_n is the FEM solution of the auxiliary linear problem $Sz_n = T(u_n) - g$, $z_{n|\partial\Omega} = 0$ in the subspace V_h. Similar to subsection 29.4.1, now the achieved (mesh independent) condition number and corresponding convergence factor, respectively, are

$$cond(F_G) = cond(S^{-1}T) \le \frac{M}{m}\,, \qquad q = \frac{M-m}{M+m}$$

where $M \ge m > 0$ are the spectral bounds in (29.16). This means that (29.13) and (29.14) are further improved when, using the weight $G(x)$, these spectral bounds m and M are closer than the original ones μ_1 and μ_2.

Altogether, we can consider (29.18) or (29.20) as weighted Sobolev gradients. This yields a finite and mesh independent condition number for any weight $G(x)$ in the given class, in contrast to $cond(T) = \infty$. Looking for $G(x)$ as a uniform approximation of the Jacobians of f, the corresponding preconditioning operator S can produce better conditioning properties than the special case $-\Delta$. For instance [92], the coefficients of S may be separable, or may contain an initial scalar coefficient or an initial Jacobian as in the modified Newton method ; see [61] for other realizations. The reader is referred to [115, 116] for further discussions and applications of weighted Sobolev gradients.

29.5 Variable Preconditioners: Sobolev Gradients with Variable Inner Product

29.5.1 Quasi-Newton Methods as Variable Steepest Descent

Now we generalize the process of subsection 29.4.2 by allowing the stepwise change of the inner products (29.15) during the iteration: in this way variable

Sobolev gradients can be constructed. (See [125, 174] for some related ideas.) In this study we will use the weak form of the elliptic operators.

Assume that the nth term of the iterative sequence is constructed, and let $G_n \in L^\infty(\Omega, \mathbf{R}^{N\times N})$ be a symmetric matrix-valued function which is spectrally equivalent to the current Jacobian, i.e.

$$m_n\, G_n(x)\xi \cdot \xi \le \frac{\partial f}{\partial \eta}(x, \nabla u_n(x))\, \xi \cdot \xi \le M_n\, G_n(x)\xi \cdot \xi \tag{29.21}$$

with constants $M_n \ge m_n > 0$ independent of $x \in \Omega$, $\xi \in \mathbf{R}^N$. The matrix $G_n(x)$ defines the weighted inner product

$$\langle u, v\rangle_{G_n} := \int_\Omega G_n(x)\, \nabla u \cdot \nabla v \tag{29.22}$$

in $H_0^1(\Omega)$.

The relation of (29.22) to the original inner product (29.8) is as follows. Endowing $H_0^1(\Omega)$ with (29.8) we can define a linear operator

$$B_n : H_0^1(\Omega) \to H_0^1(\Omega)$$

by

$$\langle B_n h, v\rangle_{H_0^1} = \int_\Omega G_n(x)\, \nabla h \cdot \nabla v \qquad (h, v \in H_0^1(\Omega)). \tag{29.23}$$

Then (29.22) is the energy inner product of B_n.

Let F denote the generalized differential operator (29.9) in the original inner product. By (29.10), F is the H_0^1-gradient of ϕ. Then the gradient ϕ'_{G_n} w.r.t. the inner product (29.22) is related to F by the relation

$$\phi'_{G_n}(u) = B_n^{-1} F(u) \qquad (u \in H_0^1(\Omega)), \tag{29.24}$$

which follows by a similar consideration as (29.20).

Corresponding to the gradients (29.24), we can define a variable gradient (steepest descent) method for problem (29.1) in V_h such that in the nth step the gradient of ϕ is taken w.r. to the inner product $\langle ., .\rangle_{G_n}$. In virtue of (29.22)-(29.23), we thus obtain the variably preconditioned sequence $(u_n) \subset V_h$:

$$\begin{aligned} u_{n+1} &= u_n - \tfrac{2\tau_n}{M_n + m_n}\, z_n\,, \\ \text{where } \langle B_n z_n, v\rangle_{H_0^1} &= \langle F(u_n), v\rangle_{H_0^1} - \langle g, v\rangle \quad (\forall v \in V_h) \end{aligned} \tag{29.25}$$

and $0 < \tau_n \le 1$ is a suitable damping parameter. As proved in [91], we can obtain the following condition numbers and convergence factor:

$$\mathit{cond}\left(B_n^{-1} F'(u_n)\right) \le \frac{M_n}{m_n} \quad (n \in \mathbf{N}), \qquad q = \limsup \frac{M_n - m_n}{M_n + m_n}\,, \tag{29.26}$$

in particular, superlinear convergence can be obtained (up to quadratic order) and its speed is determined by the rate as $M_n/m_n \to 1$.

As shown by the construction and reflected by the convergence result, the above-defined variable steepest descent iteration can alternatively be considered as a quasi-Newton method since B_n is an approximation of the derivative $F'(u_n)$.

Efficient realizations are obtained e.g. if B_n is an elliptic operator with piecewise constant coefficients (developed in the same paper [91]) or an operator with diagonal coefficients [7].

29.5.2 Newton's Method as an Optimal Variable Steepest Descent

The above discussion on variable preconditioners allows us to regard Newton's method as an optimal descent in a wider sense than for a usual gradient method. This idea has been suggested in [94] in a Hilbert space setting. We now present it for the Dirichlet problem (29.1).

The usual gradient method defines an optimal descent direction when a fixed inner product is used. In contrast, let us now extend the search for an optimal descent direction by allowing the stepwise change of inner product. For the latter the possible choices are as above in the weighted form (29.22), where G_n satisfies (29.21) with some $M_n \geq m_n > 0$, and hence (29.22) is equivalent to the usual H_0^1 inner product. As mentioned after (29.26), the resulting convergence properties are determined by the quotients M_n/m_n as $n \to \infty$.

The choice

$$G_n(x) := \frac{\partial f}{\partial \eta}(x, \nabla u_n) \quad \text{or} \quad B_n := F'(u_n),$$

which generates the inner product

$$\langle v, z\rangle_{G_n} := \int_\Omega \frac{\partial f}{\partial \eta}(x, \nabla u_n)\, \nabla v \cdot \nabla z$$

for the nth step Sobolev gradient, is an extreme case of variable preconditioner that yields optimal spectral bounds $m_n = M_n = 1$ in (29.21). Then the corresponding variable steepest descent iteration becomes the damped Newton method with quadratic convergence, moreover, in [94] we have proved that the resulting minimal value of ϕ along the search direction z_n is optimal up to second order as u_n approaches the solution.

Roughly speaking, this means that the descents in the gradient method are steepest w.r. to different directions, whereas in Newton's method they are steepest w.r. to different directions and inner products.

Remark 29.3. (i) The Newton iteration is often coupled with inner iterations for the linearized equations. The Sobolev gradient idea for these linear problems is the special case of the previous considerations when applied to the quadratic functional. Namely, let us consider the auxiliary linear equation in the nth outer Newton step:

$$F'(u_n)p = -(F(u_n) - b) \tag{29.27}$$

for which the corresponding quadratic functional is

$$\phi(p) = \frac{1}{2}\langle F'(u_n)p, p\rangle + \langle F(u_n) - b, p\rangle.$$

For the Dirichlet problem (29.1) this takes the form

$$\phi(p) = \frac{1}{2}\int_\Omega \frac{\partial f}{\partial \eta}(x, \nabla u_n)\, \nabla p \cdot \nabla p + \int_\Omega \big(f(x, \nabla u_n) \cdot \nabla p \; - gp\big)\,. \tag{29.28}$$

Then a preconditioned form of (29.27) can be defined as

$$B_n^{-1}F'(u_n)p = -B_n^{-1}(F(u_n) - b) \tag{29.29}$$

with the operator (29.23), and this corresponds to the Sobolev gradient of the quadratic functional (29.28) w.r. to the inner product (29.22). Concerning the convergence of inner iterations, note that here n is fixed. If assumption (29.21) is satisfied, then,

$$cond\left(B_n^{-1}F'(u_n)\right) \le \frac{M_n}{m_n}$$

and, accordingly, the CG iteration for (29.29) converges with ratio

$$\frac{\sqrt{M_n} - \sqrt{m_n}}{\sqrt{M_n} + \sqrt{m_n}}.$$

Here the same realizations for B_n are relevant as in subsection 29.4.2 for weighted Sobolev gradients. For instance, preconditioning operators with piecewise constant coefficients have been efficiently used in [6] in this context.

(ii) Alternative interpretations of Newton's method in Sobolev gradient context use minimization subject to constraints, see Chapter 9 and [94].

29.6 Mixed Problems and Other Extensions

In our presentation, for simplicity, we have considered a Dirichlet problem where both the original and preconditioning operators have only principal parts. However, the results of sections 29.4 and 29.5 can be extended in essentially the same form to mixed problems where both the original and preconditioning operators also contain lower order terms:

$$\begin{cases} T(u) \equiv -\mathrm{div}\, f(x, \nabla u) + q(x,u) = g(x) & \text{in } \Omega \\ Q(u) \equiv \quad f(x, \nabla u) \cdot \nu + s(x,u) = \gamma(x) & \text{on } \Gamma_N \\ \qquad\qquad\qquad\qquad u = 0 & \text{on } \Gamma_D \end{cases} \tag{29.30}$$

where the measurable subparts Γ_N, Γ_D yield a nonoverlapping decomposition of $\partial\Omega$ and, in addition to Assumptions 29.2.1, we assume that the functions q and s have similar smoothness as f and are nondecreasing w.r.t. u such that their growth is limited by the Sobolev embeddings of $H^1(\Omega)$ to $L^p(\Omega)$ and $L^p(\Gamma_N)$. (See e.g. [93] for such precise general conditions that allow well-posedness in $H^1(\Omega)$ via a convex potential.) Further, the preconditioning operator (29.19) can be modified to

$$Su \equiv -\mathrm{div}\,(G(x)\nabla u) + h(x)u, \tag{29.31}$$

where $h \in L^\infty(\Omega)$ and $h \geq 0$, defined formally for $u \in H^2(\Omega)$ with $G(x)\nabla u \in H^1(\Omega)$ and satisfying the boundary conditions

$$Ru \equiv \partial_{G(x)\cdot\nu} u + \beta(x) u = 0 \quad (x \in \Gamma_N), \qquad u = 0 \text{ on } \Gamma_D \tag{29.32}$$

(where $\partial_{G(x)\cdot\nu} u = G(x)\, \nu \cdot \nabla u$ is the conormal derivative of u at x). Based on [61, Ch. 7.], the convergence results used in section 29.4 remain valid in this case with the modification that the constant M in the convergence factor becomes some M_0 that depends suitably on the norm of the initial iterate u_0. In section 29.5 the constant M_n also becomes larger in the convergence factor but this change is independent of $p_0^{(n)}$ within an inner iteration circle to find p in (29.29). A practically most relevant case of (29.31) is a Helmholtz-like operator

$$Su \equiv -\Delta u + cu$$

with some constant $c > 0$, coupled with boundary conditions $\partial_\nu u + \beta u = 0$ on Γ_N with some constant $\beta \geq 0$. This corresponds to the Sobolev gradient w.r.t. the H^1-inner product

$$\langle u, v \rangle := \int_\Omega (\nabla u \cdot \nabla v + cuv) + \int_{\Gamma_N} \beta uv.$$

Here a large value of c improves the conditioning of the auxiliary problems.

More generally, similar ideas can be used for systems such that the preconditioning operator is an r-tuple of uncoupled elliptic operators where r is the number of equations, see also [61, Ch. 7.]. For instance, for Dirichlet problems, the r-tuple of componentwise Laplacians

$$Su = \big(-\Delta u_1, \cdots - \Delta u_r\big),$$

as preconditioning operator, corresponds to the Sobolev gradient w.r.t. the standard $H_0^1(\Omega)^r$-inner product

$$\langle u, v\rangle = \sum_{i=1}^{r} \int_{\Omega} \nabla u_i \cdot \nabla v_i$$

(see [8, 95] in the context of Newton-like or gradient type iterations, respectively). Another more general setting where the preceding ideas can be applied by suitable modifications are nonlocal boundary value problems [90].

Let us finally consider the following special case of (29.30):

$$\begin{cases} -\Delta u + q(x,u) = g(x) & \text{in } \Omega \\ \partial_\nu u = 0 & \text{on } \Gamma_N \\ u = 0 & \text{on } \Gamma_D \end{cases} \tag{29.33}$$

which is closest to the setting of Chapter 11 to determine weak solutions. Here, as for (29.30), we have assumed that the function q is nondecreasing w.r.t. u, hence (29.33) has a unique weak solution, which is the minimizer of the functional

$$\phi(u) = \int_{\Omega} \Big(\frac{1}{2}\,|\nabla u|^2 + Q(x,u) - gu\Big)$$

where Q is a primitive of q w.r.t. u. However, for such problems it is possible to get rid of the convexity of ϕ and find multiple solutions of the corresponding semilinear equation by suitably modified Sobolev steepest-descent algorithms, see Chapter 27 and [133]. Such results are promising for the possible extension of the methods of this paper beyond the coercive setting.

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Chapter 30
More Results on Sobolev Gradient Problems

Following are some brief summaries of work related to Sobolev gradients. In the past twelve years, since the first edition of this work appeared, there have been many papers concerning both theory and applications of Sobolev gradients. A complete account is beyond what this writer will undertake and apologies are offered to authors of work not cited. To partially make up for this omission, a reader interested in exploring the extent of the Sobolev gradient literature might use internet search. I have found it useful to do "Sobolev gradients" (be sure to include the quotes) or "Sobolev gradient" on google.com or scholar.google.com. Putting in names of references in this section or references in the rest of this book leads to many other papers. The term "Sobolev gradient" has by now become a generic term, with many using it who seem unaware of the term's origin (coined by this writer in the 1980's).

30.1 Singular Boundary Value Problems

Work of W.T. Mahavier [115–118] uses weighted Sobolev spaces in an interesting and potentially far reaching way. This work stems from an observation that for the singular problem

$$ty'(t) - y(t) = 0,\ t \in [0,1]$$

the Sobolev gradient constructed according to previous chapters performs rather poorly. It is shown that a Sobolev gradient taken with respect to a finite dimensional version of

$$\|f\|_W^2 = \int_0^1 [(ty'(t))^2 + (y(t))^2]\, dt$$

gives vastly better numerical performance using discrete steepest descent. It is shown how to choose weights appropriate to singularities so that the resulting

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Sobolev gradients have good convergence properties. Generalizations to systems is made in this work, which should be consulted for details and careful numerical comparisons. In Chapter 9, as part of an inquiry into metric choice, it is indicated that Riemannian metrics lead to Newton's method. In one sense this gives an optimal metric (but often not from a programmer's point of view) for descent problems associated with differential equations. The discussion there, together with references in that section, might lead to further useful metrics for singular problems. Generally, singular problems have not yet received the attention they deserve. This is a particularly interesting area for further research.

30.2 Quantum Mechanical Calculations

In [58] there is a very recent discussion of the dynamics of gases in controlled geometries, in particular of Bose-Einstein condensates in rotating traps. It is asserted there that an approximation using the Gross-Pitaevskii is sufficient for these purposes. Sobolev gradient calculations are used in this work to good effect. This thesis will certainly result in a number of journal publications.

In [185] there is also recent work relating to the nonlinear Schrödinger equation and to propagation pulses in optical fibers and also extensive work on Ginzburg-Landau functionals. The authors are here particularly interested in time evolution problems associated with this functional.

García-Ripoll and Pêrez-García in [205] deal with various problems in quantum mechanics from the point of view of Sobolev gradients. One of the problems they consider is that of finding critical points to a nonlinear Schrödinger problem of the form

$$E(\psi) = \frac{1}{2}\int \{|\nabla\psi)|^2 + \bar{\psi}[V(x) + \frac{1}{2}g|\psi|^2 - \Omega L_z]\psi\} d^n x, \tag{30.1}$$

where the integration is over R^n and $\psi \in L_2(R^n, C)$. Given a positive integer N, they impose the condition

$$\int |\psi|^2 = N \tag{30.2}$$

on prospective critical points on (30.1). Instead of a finite difference or finite element setting, the authors use linear combinations of a Fourier basis for an appropriate bounded computational region in R^n. They arrive at a Sobolev gradient $\nabla_S E$ of the form

$$(\nabla_S E)(\nu) = (I - \Delta)^{-1}[-\frac{1}{2}\Delta + V(x) + g|\nu|^2 - \Omega L_z]\nu,\ \nu \in L_2(R^n, C).$$

They apply their considerations to a problem in nonlinear optics and indicate that their Sobolev gradient implementation gives about two orders of magnitude improvement over more conventional methods.

There is a great deal of current work on numerical and theoretical Gross-Pitaevskii and Ginzbug-Landau energy functionals, much of it using Sobolev gradients and concerned with preserving (30.2) under iterations.

This writer has had many discussions recently with a number of researchers on these problems. For various reasons it is best to not attempt a discussion here of these works in progress, one reason being that papers have just been submitted for publication. Suffice it to say that the interested reader might keep abreast of research appearing by P. Kazemi, M. Eckart, S. Sial, N. Raza, S. Siddiqi, J. Garcia-Ripoll and authors to which they refer, among others.

30.3 Dual Steepest Descent

Suppose that each of H, K, S is a Hilbert space, F is a $C^{(1)}$ function from H to K and B is a $C^{(1)}$ function from S to R. Denote by ϕ, ψ, η the functions on H defined by

$$\phi(x) = \|F(x)\|_K^2,\ x \in H,$$
$$\psi(x) = \|B(x)\|_S^2,\ x \in H.$$
$$\eta = \phi + \psi.$$

Dual steepest descent, used by Richardson in [196,198], consists in seeking $u \in H$ such that

$$u = \lim_{t\to\infty} z(t) \text{ and } F(u) = 0, B(u) = 0 \tag{30.3}$$

where

$$z(0) = x \in H,\ z'(t) = -(\nabla\eta)(z(t)),\ t \geq 0. \tag{30.4}$$

The following is a convergence result from [196]. All inner products and norms in this section without subscripts are to be taken in H.

Theorem 30.1. *Suppose Ω is an open subset of H, z satisfies (30.4) and $R(z) \subset \Omega$. Suppose also that there exists $c, d > 0$ such that*

$$\|(\nabla\phi)(y)\| \geq c\|F(y)\|_K, \|(\nabla\psi)(y)\| \geq d\|B(y)\|_S,\ y \in \Omega.$$

Finally suppose that there is $\alpha \in (-1, 1]$ so that if $y \in \Omega$, then

$$\langle(\nabla\phi)(y), (\nabla\psi)(y)\rangle/(\|(\nabla\phi)(y)\|\ \|(\nabla\psi)(y)\|) \geq \alpha.$$

Then there is z such that (30.4) holds.

Proof. (From [196]) Clearly one may assume that $\alpha \in (-1, 0)$. Then

$$\begin{aligned}
\|(\nabla\eta)(y)\|^2 &= \|(\nabla\phi)(y) + (\nabla\psi)(y)\|^2 \\
&= \|(\nabla\phi)(y)\|^2 + 2\langle(\nabla\phi)(y), (\nabla\psi)(y)\rangle + \|(\nabla\psi)(y)\|^2 \\
&\geq \|(\nabla\phi)(y)\|^2 + 2\alpha\|(\nabla\phi)(y)\| \, \|(\nabla\psi)(y)\| + \|(\nabla\psi)(y)\|^2 \\
&= -\alpha[\|(\nabla\phi)(y)\|^2 - 2\|(\nabla\phi)(y)\|\|(\nabla\psi)(y)\| + \|(\nabla\psi)(y)\|^2] \\
&+ (1+\alpha)[\|(\nabla\phi)(y)\|^2 + \|(\nabla\psi)(y)\|^2] \\
&\geq (1+\alpha)\min(c^2, d^2)[\|F(y)\|^2 + \|B(y)\|^2] \\
&= (1+\alpha)\min(c^2, d^2) 2\eta(y).
\end{aligned}$$

The conclusion (30.3) then follows from Theorem 4.4 of Chapter 4. □

30.4 Optimal Embedding Constants for Sobolev Spaces

This section reports on work of Richardson in [198]. It is known, for example, (see [2]), that if n is a positive integer, then the Sobolev space $H^{n,2}$ is compactly embedded into $C([0,1])$, that is, there is $c > 0$ such that if $f \in H^{n,2}$, then

$$c\|f\|_{H^{n,2}} \geq \|f\|_{C([0,1])}. \tag{30.5}$$

There is considerable interest in determining this constant, as well as similar constants for other pairs of spaces (cf [109, 120, 217] for example). In [198], an explicit expression is given for this the number c in (30.5), namely

$$c = \left\{ (\frac{2}{n+1} \sum_{k=1}^{n} \frac{(\sin(k\theta))^2}{\tanh(sin(k\theta))} \right\}^{\frac{1}{2}}$$

A primary feature of an argument for this result is the use of the adjoint operator for the linear functional L from $H^{n,2}$ into R defined, for some $a \in [0,1]$, by

$$Lf = f(a), \ f \in H^{1,2}([0,1]).$$

Work in [198] eventually inspired the development in Chapter 8 in which orthogonal projections onto various null spaces of linear functionals were constructed in connection with boundary value problems.

30.5 Performance of Preconditioners and H_{-1} Methods

References [199–203] by Richardson contain insightful comparisons of different variations on Sobolev gradients. For an indication of H_{-1} see (5.14). In [202], Richardson gives an example of a system of two partial differential equations for which a least-squares formulation has one equation in an L_2 norm and the other in the corresponding H_{-1} norm. He discusses his motivation for this and explains how this is related to Sobolev gradients (see [202] and also [71] for details).

In Section 4 of [202] Richardson considers the simple problem of finding u such that

$$-u'' = 1,\ u(0) = 0 = u(1).$$

For a discrete version of this problem, Richardson plots the ordinary gradient and the finite dimensional gradients corresponding to $H^{1,2}([0,1])$ and to $H^{2.2}([0,1])$ respectively. This last space is the right one. The first gradient, that is the ordinary one, is very rough, the second gradient is much less so but the third one is smooth and does by far the best of the three in reaching a solution to the problem. He reconfirms results in Chapter 2 in which convergence is terminally slow for the wrong gradient but fast for the correct one. Here there is an intermediate space, $H^{1,2}([0,1])$, with decidedly intermediate convergence results. In [199] there is an indication that a Courant-Frederichs-Lewy condition is consistent with step size choice in following continuous steepest descent numerically. In that paper there are additional H_{-1} results.

30.6 Poisson-Boltzmann Equation

In [201] Richardson gives a treatment, using Sobolev gradients, of a Poisson-Boltzmann equation:

$$\nabla \cdot (\epsilon_s \nabla \phi) = -q[n_0 \exp(-\phi(x)/V_r) - n_0 \exp(\phi(x)/V_r) + N_{net}] \qquad (30.6)$$

for the study of semiconductor devices. A numerical study indicates vastly fewer, by several orders of magnitude, iterations using Sobolev gradients as compared with using an ordinary gradient. Actually a whole family of Poisson-Boltzman equations are shown to lead to similar results. This paper is highly recommended for those interested in semiconductor properties.

Robert Renka, Sultan Sial and the present writer wrote codes for some Poisson-Boltzman equations to study transport in organic diodes. These have not yet been submitted for publication.

30.7 Time Independent Navier-Stokes

In [16] Beasley uses finite elements to construct Sobolev gradients in connection with problems for Burgers' equation and the time-independent Navier-Stokes equations. He illustrates his techniques on Burgers' equation and goes on to treat a square cavity problem in which there is a open top with a constant velocity fluid passing over it. Additional finite element calculations are found in [108].

30.8 Steepest Descent and Hyperbolic Monge-Ampere Equations

A typical Monge-Ampere equation on a region Ω in R^2 may be written as the problem of finding $u \in H^{2,2}(\Omega)$ so that

$$u_{1,1}u_{2,2} - u_{1,2}u_{2,1} = f, \tag{30.7}$$

where $f \in L_2(\Omega)$ is a given function. If $f > 0$ on Ω, then any solution u to (30.7) is elliptic at each point of Ω. To see this, define $F : H^{2,2}(\Omega) \to L_2(\Omega)$ by

$$F(u) = u_{1,1}u_{2,2} - u_{1,2}u_{2,1},\ u \in H^{2,2}(\Omega)$$

and note that if $h \in H^{2,2}(\Omega)$, then

$$F'(u)h = u_{1,1}h_{2,2} + h_{1,1}u_{2,2} - u_{1,2}h_{2,1} - h_{1,2}u_{2,1},\ h \in H^{2,2}(\Omega).$$

The condition that $F(u) > 0$ is precisely the condition for the differential operator $F'(u)$, and hence a solution u to (30.7), be elliptic. But then if $f > 0$, a solution u to (30.7) must be elliptic. A great deal is known about elliptic Monge-Ampere equations (see in particular [28]). However, much less is known about hyperbolic Monge-Ampere equations, those in which f in (30.7) is negative. If f is positive on part of Ω and negative on another part, then any solution u to (30.7) is elliptic in some part of Ω and hyperbolic in another part. Very little is known about what supplementary conditions for Monge-Ampere equations, in non-elliptic cases, might be necessary and sufficient for existence and uniqueness of solutions.

Recent work of Tamani Howard begins to shed light on hyperbolic Monge-Ampere equations. As was shown in Chapter 15, in the vastly simpler case of the Tricomi equation, the theory of Sobolev gradients gives a possibility of investigating solutions to equations for which boundary conditions are not understood. Chapters 19,20 have a possibility of being relevant to both Tricomi and Monge-Ampere equations, but that has yet to come about.

Howard in [84], in a ground-breaking work, shows convergence of continuous steepest descent to a solution to (30.7) for cases in which $f < 0$. She has a local existence result in the sense that if steepest descent is started near enough to a solution, then it converges to some solution. She also presents MatLab codes which numerically calculate zeros to a finite dimensional version of (30.7). As in the Tricomi equation, her codes permit experimentation with various possible boundary conditions.

30.9 Application to Differential Algebraic Equations

An example of a differential algebraic equation (DAE) is given by the following: Suppose n is a positive integer and each of A, B is in $L(R^n, R^n)$. Consider the problem of finding solutions $Y : [0,1] \to R^n$ to

$$AY' = BY. \tag{30.8}$$

If A has an inverse, then (30.8) is equivalent to

$$Y' = A^{-1}BY, \tag{30.9}$$

an elementary problem for a first course in differential equations. However, if A fails to have an inverse, then (30.8) is another matter entirely. In particular, it is not so clear what a basis for solutions is in this case, in distinction to (30.9) in which n solutions starting at zero with n independent vectors for initial conditions is sufficient to provide a basis for all solutions of this equation. Nonlinear or inhomogeneous versions of (30.8) considerably add to this difficulty. To see that equations such as (30.8) are substantial, it is pointed out that equations whose solutions provide circuit simulators are of this type (see [31] for a through discussion).

In [172] there is a ground-breaking development, by Robin Nittka and Manfred Sauter, applying Sobolev gradients to the problem of finding a basis for solutions to DAE of a type for which (30.8) is a representative. Their approach is illustrated for this last equation. Define

$$\phi : H = H^{1,2}([0,1]) \to K = L_2([0,1])$$

by

$$\phi(Y) = \frac{1}{2}\|AY' - BY\|_K^2.\ Y \in H.$$

Compute a Sobolev gradient for ϕ, or rather for an finite dimensional version of ϕ. Run steepest descent for a variety of initial estimates to Y. Take the resulting collection of solutions and sort them carefully to determine a basis (this is not so easy when dealing with numerics since just about any set of vectors (of size less than n) in an n dimensional space can appear to be independent). The values at zero of such a basis provide the set of all possible initial values for (30.8), at least if a sufficient number of initial starts Y are chosen for steepest descent. I believe that the work [172] provides a solid basis for a new generation circuit simulator. It would take a great deal of development, but I think it can be forthcoming.

30.10 Control Theory and PDE

In Chapter 8 it is noted that a system of PDE together with supplementary conditions may be written as (8.3):

$$(\nabla\phi)(u) = 0 \text{ and } B(u) = 0. \tag{30.10}$$

In [183], B. Protas gives a related, but more general formulation of such problems in the language of control theory. He cites [1,76,112] for background on control theory. For now, the discussion is restricted to a Hilbert space setting although that is not necessary (see [183], for more details on this point). Given Hilbert spaces H and S and functions $F, G : H \times S \to R$, find $x \in H, q \in S$ so that

$$F(x, q) \text{ is minimum subject to } G(x, q) = 0. \tag{30.11}$$

The space H is called a state space and the space S is called a control space. Protas notes that in many instances, there is a function $p : S \to H$ so that if $G(x, q) = 0$, then $x = p(q)$. In such a case define $\phi : S \to R$ by

$$\phi(q) = F(p(q), q),\ q \in S.$$

Then the problem (30.11) may be rewritten as the problem of finding a relative minimum q of ϕ.

Protas' paper [183] contains an excellent discussion of gradient choice for a variety of PDE problems. Some of his discussion mirrors issues (Chapters 8,10,12), brought up in the present volume but his discussion in a number of areas breaks new ground. A reader is encouraged to consult [183] for this discussion, but might want to look at Chapter 18 first.

Developments in [183] are illustrated with the Kuramoto-Sivashinksy equations. For q in an appropriate control space:

$$\begin{cases} \partial_t u + 4\partial_x^4 + \kappa(\partial_x^2 + u\partial_x u) = 0,\ x \in \Omega,\ t \in [0, T] \\ \partial_x^i u(0, t) = \partial_x^i u(2\pi, t),\ t \in [0, T],\ i = 0, 1, 2, 3, \\ u(x, 0) = q,\ x \in \Omega. \end{cases}$$

The control q is the initial value for the system. This is a more significant example than the simple one in Chapter 18. Here also a time-dependent equation with spatial dimension n may be considered as an optimization problem in dimension $n + 1$. This can be computationally extravagant in a numerical setting but in this writer's opinion may be useful in situations where governing equations may lead to chaos but also a form of chaos may be an artifact of discretization. In some cases it is important to try to sort out the two forms of chaos.

The Kuramoto-Sivashinsky equations serve as a motivation for a discussion of Navier-Stokes equations. A problem under consideration is that of coefficient identification for such a system. A least squares equation is constructed in which coefficients are determined by optimizaton. Such considerations are highly relevant to systems of PDEs which attempt to model weather. This writer has held discussions with Andrew Bennett concerning the possibility of using Sobolev gradient methods to chose coefficients in Navier-Stokes like systems starting with actual weather data (see [17]), but nothing definitive has yet resulted.

In [183], in connection with the problem of gradient selection in connection with optimization for PDEs, Protas deals with Besov spaces as places in which gradients might lie. The paper reports a substantial variety of numerical results comparing performance of various gradients. The paper concludes with a discussion of preconditioners which might be read in connection with Chapter 29.

30.11 An Elasticity Problem

In [51] Dix and McCabe consider the problem of finding critical points of

$$\phi(u) = \int_{\Omega} [\|\nabla(u)\|^2 + (det(\nabla(u))^{-1/2}],\ u \in H^{1,2}(\Omega, R^3), \qquad (30.12)$$

where Ω is a bounded region in R^3 and $\nabla(u) : \Omega \to L(R^3, R^3)$ is the matrix valued representation of u'. Members $u \in H^{1,2}(\Omega, R^3)$ which are a critical points of ϕ are sought so that the determinants in (30.12) are nonnegative. A Sobolev gradient for ϕ is constructed and critical points of it are found numerically. See [51] for more references and details.

30.12 A Liquid Crystal Problem

In [70], Garza deals with the problem of numerically determining critical points of

$$E(u) = \int_{\Omega} |\nabla u|^2 \qquad (30.13)$$

where for some ρ in $(0, 1)$,

$$\Omega = \{(x, y, z) \in R^3 : \rho^2 \leq x^2 + y^2 \leq 1, 0 \leq z \leq 1\}$$

and $u \in H^{1,2}(\Omega, R^3)$ is subject to the condition that

$$\|u(x, y, z)\| = 1, (x, y, z) \in \Omega \tag{30.14}$$

and $u(x, y, z)$ be normal to the boundary of Ω for all $(x, y, z) \in \partial\Omega$.

According to [19], for ρ small enough there are two critical points to (30.13), one being a trivial one and the other being considerably more interesting. In [70] there is determined numerically a Sobolev gradient for finding critical points of (30.13). A unique feature of this gradient is that it respects (30.14) in the sense that continuous steepest descent preserves this condition. In [19], the full symmetry of Ω is required. On the other hand, Garza's numerical method does not depend on any particular symmetry of Ω. It thus seems appropriate for design purposes on regions of various shapes. This is a ground-breaking work. So far as the present writer knows, this is the only instance in which a Ginzburg-Landau without a penalty term such as

$$\frac{\kappa^2}{4}|u^2 - 1|^2.$$

has been treated numerically. For this problem (30.14) is enforced by building it into the relevant Sobolev gradient. Many other significant problems could be treated in this way. See [70] for details.

30.13 Applications to Functional Differential Equations

Although it hasn't been emphasized in this volume, many of the existence results of Chapters 3,4 are applicable to functional differential equations (FDEs, see [77] for a general reference). A particular example is the following: Suppose that $f, g \in C^1(R)$. Find $u : R \to R$ so that

$$u'(t) = (f \circ g)(t),\ t \in R$$

where $f \circ g$ denotes the composition of f and g. In [207] there are results for equations of the form

$$u'(t) = F(t, u(g(t))),\ t \in R.$$

These are representative of a vast, largely unexplored class of non-local problems, problems in which a derivative of an unknown at some point of the domain of the solution depends on the value of the unknown at some other point, for instance. Of course problems may be much more complicated: the value of the derivative at some point might depend on values of the unknown at many points. Partial FDEs could show immense variety. Existence results for this equation are obtained using contraction mappings but these problems are readily expressed using least squares and hence Sobolev gradients may be used.

In [146] there are applications of results in Chapter 3. A representative result is the following:

Theorem 30.2. *Suppose that P is the orthogonal projection of $L_2(R)^2$ onto*

$$\{\begin{pmatrix} u \\ u' \end{pmatrix} : u \in H^{1,2}(R)\},$$

$\alpha < 0, \beta > 0$ and r, s are bounded measurable functions on R. If $f, g \in L_2(R)$, define

$$A\begin{pmatrix} f \\ g \end{pmatrix} = g + rf_\alpha + sf_\beta$$

where if $\gamma \in R$ then $f_\gamma(t) = f(t+\gamma),\ t \in R$. Denote by L the orthogonal projection of $L_2(R)^2$ onto the range of A. If $f, g \in L_2(R)^2$,

$$\begin{pmatrix} u \\ u' \end{pmatrix} = \lim_{n\to\infty} (PLP)^n \begin{pmatrix} f \\ g \end{pmatrix}$$

exists, u satisfies

$$u' + ru_\alpha + su_\beta = 0$$

and is the solution to this equation so that $\binom{u}{u'}$ is the nearest element in $L_2(R)^2$ to $\binom{f}{g}$.

Additional numerical and theoretical results on FDE by Bakker are found in [12]. This work is related to Chapter 21.

30.14 More About Active Contours

In [216], there is a description on how Sobolev gradients give much more favorable flows than do conventional gradients do for tracking applications and both edge-based and region-based models.

In [15], there is an announcement for a poster on 'Sobolev Gradients and Neural Networks' by Bastian, Gunther and Moon. Details not available as of this writing.

30.15 Another Solution Giving Nonlinear Projection

Suppose that each of H and K is a Hilbert space and $F : H \to K$ is a $C^{(2)}$ transformation such that

$$(F'(x)F'(x)^*)^{-1} \in L(K, K),\ x \in H$$

and $F(0) = 0$.

Denote by P, Q functions on H such that if $x \in H$, then $P(x)$ is the orthogonal projection of H onto the null space of $F'(x)$ and $Q(x) = I - P(x)$. Denote by f, g the functions on $R \times H \times H$ to H such that if $x, \lambda \in H$ then

$$f(0, x, \lambda) = x,\ f_1(t, x, \lambda) = P(f(t, x, \lambda))\lambda,\ t \geq 0,$$

and

$$g(0, x, \lambda) = x,\ g_1(t, x, \lambda) = Q(g(t, x, \lambda))\lambda,\ t \geq 0.$$

Define M from H to H so that if $\lambda \in H$ then

$$M(\lambda) = g(1, f(1, 0, \lambda), \lambda).$$

The following is due to Lee May [121].

Theorem 30.3. *There is an open subset V of H, centered at $0 \in H$ such that the restriction of M to V is a diffeomorphism of V and $M(V)$ is open.*

Denote by S the inverse of the restriction of M to V and denote by G the function with domain S so that

$$G(w) = f(1, 0, S(w)),\ w \in R(M).$$

The following is also from [121] and concerns the function G fo the previous theorem:

Theorem 30.4. *$R(G) \subset N(F)$.*

The function G is a solution giving nonlinear projection. Two elements $x, y \in D(S)$ are said to be equivalent if $G(x) = G(y)$. Arguments in [121] use an implicit function and are essentially constructive. Thus G associates each element near enough to 0 with a solution. Many of the comments about the function G in Chapter 19 apply as well to the present function G. The reader might consult [121] for careful arguments for the two results of this section.

30.16 Dynamics of Steepest Descent

In [87] Jon Jacobsen compares, for a given functional ϕ, the dynamics of Sobolev gradient and conventional steepest descent. In one of his examples he considers

$$\phi(u) = \int_0^1 (u')^2,\ u \in H_0^{1,2}([0,1]).$$

Conventional steepest descent leads to the well-known heat equation. In contrast, the Sobolev gradient $\nabla_S\phi$ is given by

$$(\nabla_S\phi)(u) = u,\ u \in H^{1,2}([0,1]).$$

Consequently, Sobolev gradient steepest is given by $z : [0,\infty) \to H^{1,2}([0,1])$ so that

$$z'(t) = -z(t),\ t \geq 0. \tag{30.15}$$

It would be almost universally agreed that solutions to the heat equation track closely the actual path of temperature decay and that (30.15) is just a convenient way to go to the (sole) equilibrium position. Nevertheless it is interesting to consider how closely various gradients, chosen with respect to various metrics, are able to track time evolution.

30.17 Aubry-Mather Theory and a Comparison Principle for a Sobolev Gradient Descent

A very recent work [14] of T. Blass, R. de la Llave and E. Valdinoci uses Sobolev gradient descent to find critical points of S:

$$S(u) = \frac{1}{2}\langle u, Au\rangle_{L_2(\Omega)} + \int_\Omega V(x,u)\,dx,$$

where Ω is a region in R^n, A is a uniformly elliptic operator and u is in some appropriate Sobolev space. A Sobolev gradient for S is constructed and some convergence results are proved. Of particular interest is the use of fractional powers in an essential way.

Chapter 31
Notes and Suggestions for Future Work

Some directions for future work are indicated in this final chapter. It is hoped that a reader will at this point have their own list. Also included are some random comments.

- Many more Sobolev gradient calculations have been made with finite differences, as opposed to finite elements. This is essentially an historical accident. Further investigations using finite elements will be enlightening. So far as I know, no Sobolev gradient calculations have been made using wavelets. Surely this can be done.
- Weighted Sobolev gradients have been encountered in a number of places in the present work. They have been used in singular problems, first by W. T. Mahavier, and then others. In a different direction, weighted gradients have been used to enforce supplementary conditions. Much more investigation is indicated. Even continuous Newton's method may be interpreted as a weighted Sobolev gradient development.
- At the heart of this volume are results on convergence of continuous steepest descent. Despite considerable recent progress, this is still an open area for research. Work of Kazemi, indicated in Chapter 14, is a good starting point for further work.
- Much more work is in order showing convergence of a sequence of finite difference (or finite element) solutions to a continuous solution as meshes approach zero. I have long thought that one of the strengths of Sobolev gradient theory is that such convergence actually occurs, but rather little effort so far has gone into to this important problem.
- More examples of instances in which the Nash-Moser results of Chapter 9 apply are needed. Conditions given there are much simpler than given in the original work of Moser, [122], but very little effort has been made with applications. In [166], there is a rather involved comparison between [166] and [122], noting that a considerable portion of the hypothesis in [122] is not needed in [166]. It is indicated that symmetric hyperbolic systems seem to be covered by both, but a more involved comparison is still needed. The best approach is to tackle specific problems, keeping the requirements of both developments in mind.

J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Lecture Notes in Mathematics 1670, DOI 10.1007/978-3-642-04041-2_31,

- The function space development in Chapter 16, on minimal surfaces, needs to be put on more solid ground. Numerics in this chapter seem to work, but it is not even clear that the proper function spaces have been chosen. Using exterior derivatives, the development could be extended to all finite dimensions. Work in this chapter is prototypical of what might be attempted for other problems. In contrast with 'evolution by mean curvature', a partial differential equation, Sobolev gradients indicate an ordinary differential equation in function space. Numerical advantages of Sobolev gradients seem clear for such problems, but function space developments are barely begun. Other problems which uses partial differential equations for evolution are Nash's embedding theorem (work is in progress on this) and even a search for an alternative argument for the Poincare conjecture. More generally there is the prospect of further extending Sobolev gradient ideas to a variety of problems on manifolds.
- Vastly more work is indicated for variational problems. Many of the problems in the literature which are treated by minimizing sequences should be amenable to the constructive method of Sobolev gradients. This would open up more numerical alternatives to dealing with Euler-Lagrange equations. Chapter 14, among other developments in this volume, indicate a path for investigating a wide variety for variational problems.
- The ideas outlined in Section 10.3 are the starting place for a new theory of the spectrum of Riemannian manifolds - a theory which caries with it a natural numerical counterpart. What is given in 10.3 is just a sketch of what might be a rather comprehensive theory.
- A theory of linear multipoint supplementary condition problems for ordinary differential equations can be built as limiting cases of the development in Section 8.7. See work of Zettl, [229], for background on boundary value problems with which some of our finite developments in Chapter 8 are connected. See [135], for example, for a general function space formulation of such problems.
- Work on Sobolev gradients for non-inner product spaces, building on Chapter 16 and the work of Zahran ([227, 228]) is indicated as a possible starting point. Almost all of the developments in Chapter 4 should have a counterpart in non-Hilbert space settings. Work so far is promising, but certainly much more remains to be found.
- Work on transonic flow using Sobolev gradients was first suggested to this writer by Graham Carey after I gave a talk entitled 'a type-independent method for partial differential equations'. This led to my seeking, with my students and many others represented in this book, a succession of physical problems. After work on Carey's problem, [160], I gave talks at Boeing in the 1980's on the subject. Two test problems suggested by researchers at Boeing were solved, apparently to the satisfaction of these researchers. Graphs of some solutions appear in Chapter 17. I have had little contact with Boeing since then, but I have reason to think that my

methods have some influence there. One might try "Jameson", "Sobolev gradient", "Sobolev gradients" (using the quotes) on Google in order to help form an opinion on this matter.

- Sobolev gradient calculations seeking beneficial configurations of 'holes' and 'moats' in superconducting devices is, in the opinion of some established workers in the field, nearing the design stage. I hope that collaboration with experimentalists will lead a useable simulator. Such a simulator could allow engineers to consider a vast number of possibilities - much greater than is possible by only building and testing individual devices.
- Building on the work of Knowles, Chapter 26, one can envision useful codes for processing seismic data. Knowles' work started with an investigation of numerical differentiation. Seismic data typically is rough but rather fine subsurface details are sought. Modeling of existing oil fields is a related interesting possibility for extending Knowles' work.
- Some very promising work is being done on nonlinear Schrödinger equations using Sobolev gradients. In particular there is work by Ripoll, [205] and by Kazemi and Eckhart (being submitted for publication).
- Works of Protas, Renka and the present writer (see Chapter 18) provide a new point of view on time-dependent partial differential equations. Just enough has been done to establish the viability of this approach. A full-scale numerical attack on Navier-Stokes with the indicated method might show that some numerically perceived 'chaos' is just an artifact of using step-by-step methods. Unpublished calculations concerning compound pendulums seem to indicate that step-by-step (in time) calculations are capable of inducing apparent chaos into systems. Many of these systems have a natural chaos, but chaos artificially induced by discretizing seems to add to this natural chaos, leaving the problem of separating the two brands of chaos.
- A. Bennett suggested to me the possibility of using Sobolev gradients for data assimilation connected with weather modeling (see [17]). The idea is to use Sobolev gradients to process world-wide weather data in order to arrive at coefficients for a grand Navier-Stokes equation. The process involves finding a nearest, in appropriate Sobolev metric, numerical function which interpolates the data. The resulting Navier-Stokes equation, when solved numerically, would be used for weather prediction. This idea was influenced by Knowles' work.
- There is the matter of trying to use results of Chapter 20 to break the hold of the almost exclusive use of 'boundary conditions' as opposed to more general supplementary conditions. Various methods in partial differential equations rely upon integration by parts and hence seem to focus only on boundary conditions which cause integration by parts terms to vanish. Chapters 15, 19, 20 represent an attempt to establish a new, and likely needed, point of view on supplementary conditions. This work represents only a rather timid start, but the problem is of tremendous importance.

- Material in Chapter 22 and to some extent, Chapter 21, give a brief view of a theory from which the theory of Sobolev gradients arose. It is based on spaces of analytic functions. The hope was that one could somehow pass to a limit and so include non-analytic solutions. With a failed attempt to make the developments of Chapter 22 numerical, I switched my point of view to Sobolev spaces. As I have tried to indicate, the numerical and function space aspects of Sobolev gradients are very closely related. However, work of Pate (see references) holds promise of further valuable discoveries for the earlier analytic theory.
- The main point of this book is to encourage the pursuit of a central point of view on partial differential equations, one that encompasses existence, uniqueness, supplementary conditions, qualitative properties and numerics under one umbrella. Historically such a point of view has been achieved for the finding of roots of polynomials, then again for ordinary differential equations. It is my belief that despite almost universal skepticism on this issue, the great tide of mathematical history will carry us to a unified point of view for partial differential equations. I hope that the present work stirs things up in this direction.

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Edited by J.-M. Morel, F. Takens, B. Teissier, P.K. Maini

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