

SOBOLEV GRADIENTS: INTRODUCTION, APPLICATIONS, PROBLEMS

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ABSTRACT. Sobolev gradient is defined and a simple example is given. A number of applications are described. A number of problems are stated, some of which are open problems for research.

1. INTRODUCTION TO SOBOLEV GRADIENTS

Sobolev gradients are an efficient method of calculating solutions to a wide variety of systems of partial differential equations. Successful applications have been made to problems in transonic flow, Ginsburg-Landau equations for superconductivity, elasticity, minimal surfaces and oil-water separation problems.

A basic reference is [12]. This reference contains motivation and background for Sobolev gradients as well as applications up to the time of publication in 1997. The present paper will summarize more recent applications and will present a number of problems. Some of the problems are exercises, some are very open ended and some may be impossible.

Suppose X is a Banach space with the property that if f is a continuous linear function from X to R , then, given $c > 0$, there is a unique element $h \in X$ so that

$$\sup_{g \in X, \|g\|_X = c} fg = fh. \quad (1)$$

Such spaces X include all Hilbert spaces as well as many Sobolev spaces which are not Hilbert spaces (see [20]). If ϕ is a C^1 functional on the Sobolev space X with the above property, then the Sobolev gradient of ϕ at $x \in X$ is the element $(\nabla\phi)(x)$ so that

$$\sup_{g \in X, \|g\|_X = |\phi'(x)|} \phi'(x)g = \phi'(x)(\nabla\phi(x)).$$

Our general reference for Sobolev spaces is [1]

Given a function ϕ as above, one seeks a critical point of ϕ by either continuous or discrete steepest descent. Discrete steepest descent is the classical process of constructing a sequence $\{x_k\}_{k=0}^{\infty}$ so that x_0 is given and

$$x_k = x_{k-1} - \delta_k(\nabla\phi)(x_{k-1}), \quad k = 1, 2, \dots, \quad (2)$$

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where for each k , δ_k is chosen so that

$$\phi(x_{k-1} - \delta_k(\nabla\phi)(x_{k-1}))$$

is minimal in some appropriate sense. A critical point of ϕ is sought as

$$u = \lim_{k \rightarrow \infty} x_k.$$

On the other hand, continuous steepest descent consists of constructing a function $z : [0, \infty) \rightarrow X$ so that

$$z(0) = z_0 \in X, \quad z'(t) = -(\nabla\phi)(z(t)), \quad t \geq 0 \quad (3)$$

and then seeking $u \in X$ so that

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

so that u is a critical point of ϕ .

Continuous steepest descent provides a theoretical starting point for proving convergence of discrete steepest descent.

Functions ϕ of interest fall into two groups. The first group consists of problems in which ϕ comes from a classical variational principle, for example, ϕ is an energy functional. A critical point of such a functional ϕ is frequently a solution to a system of partial differential equations under some boundary conditions.

The second group of problems is given by a function ϕ for which there is a function F from X to a second Banach space Y so that

$$\phi(x) = \|F(x)\|_Y^2/2, \quad x \in X. \quad (4)$$

We think F as being so that a zero u of F is a solution to a system of partial differential equations. It is quite common that a critical point of ϕ is actually a zero of F , something not so common for general optimization problems. This point is discussed in some detail in [12]. Functionals ϕ of the second type are generally used only when one has a system of partial differential equations for which a conventional variational principle is not available.

For numerical computation, finite dimensional versions of functions ϕ as above are considered. The main practical point in the use of Sobolev gradients in applications is the following: If ϕ either represents a conventional variational principle or is given by (4), for ϕ to be C^1 , it must be that the norm on X is chosen properly with respect to any derivatives contained in the definition of ϕ (we are thinking here that X is a Sobolev space of functions). In finite dimensional approximations to ϕ by, say a function ϕ_n , n being the number of grid points used in an approximation, the norm on a corresponding finite dimensional space should simulate the required norm on X . An ordinary gradient of ϕ_n could be calculated (in the usual way, as a list of partial derivatives), but such a gradient is quite different from the corresponding Sobolev gradient (and has vastly inferior numerical properties). The reader might consult [12] for a detailed discussion of this point. To illustrate these comments we use the following very simple example.

Suppose X is the Sobolev space $H^{1,2}([0, 1])$ and $K = L_2([0, 1])$. Define $F : X \rightarrow K$ by

$$F(u) = u' - u, \quad u \in X. \quad (5)$$

With ϕ defined as in (4) in relation to this F , we see that zeros of ϕ are precisely the solutions u on $[0, 1]$ to

$$u' - u = 0, \quad (6)$$

these being, of course, just constants times the exponential function.

Problem 1. Show that for F as in (5) and ϕ as in (4), any critical point of ϕ is also a zero of F .

The next few problems lead to the construction of the Sobolev gradient $\nabla_S \phi$ of ϕ as defined in (4) where F is defined in (5). We denote the Sobolev gradient of ϕ by

$$\nabla_S \phi$$

to be so that

$$(\phi'(u))h = \langle h, (\nabla_S \phi)(u) \rangle_X, \quad u, h \in X.$$

Problem 2. Show that

$$(\phi'(u))h = \int_0^1 (h' - h)(u' - u), \quad u, h \in X.$$

Problem 3. Show that

$$(\phi'(u))h = \left\langle \begin{pmatrix} h \\ h' \end{pmatrix}, P \begin{pmatrix} y - y' \\ y' - y \end{pmatrix} \right\rangle_{L_2([0,1])^2} u, \quad h \in X,$$

where P is the orthogonal projection of $L_2([0, 1])^2$ onto

$$W = \left\{ \begin{pmatrix} y \\ y' \end{pmatrix} : y \in X \right\}.$$

Problem 4. Show that

$$W^\perp = \left\{ \begin{pmatrix} y' \\ y \end{pmatrix} : y \in X, y(0) = 0 = y(1) \right\}.$$

Use this fact to obtain an expression for the orthogonal projection P and hence for $\nabla_S \phi$.

We now begin some numerics. Divide the interval $[0, 1]$ into n pieces of equal length, define ϕ_n by (for $y = (y_0, y_1, \dots, y_n)$)

$$\phi_n(y) = \sum_{k=1}^n ((y_k - y_{k-1})/\alpha - (y_k + y_{k-1})/2)^2 / 2$$

where $\alpha = 1/n$. Now ϕ_n has an ordinary gradient. Discrete steepest descent as described above may be attempted using this ordinary gradient. Even though it is possible to *prove* that this process converges to a zero of ϕ_n , numerical performance is extremely poor, as documented in [12]. When using conventional

gradients for problems in differential equations, one finds such poor performance universal. We now contrast this situation with a corresponding Sobolev gradient. Note first that if $\nabla\phi_n$ denotes the ordinary gradient function, then

$$(\phi'(x))h = \langle h, (\nabla\phi_n)(x) \rangle_{R^{n+1}}, \quad x, h \in R^{n+1}.$$

The Sobolev gradient, $\nabla_S\phi_n$ is defined to be the function on R^{n+1} so that

$$(\phi'(x))h = \langle h, (\nabla_S\phi_n(x))_{S,n} \rangle_{S,n}, \quad x, h \in R^{n+1}$$

where

$$\langle *, * \rangle_{S,n} \tag{7}$$

denotes the inner product associated with the following second norm on R^{n+1} :

$$\|y\|_{S,n}^2 = \sum_{k=1}^n ((y_k - y_{k-1})/\alpha)^2 + ((y_k + y_{k-1})/2)^2,$$

$$y = (y_0, y_1, \dots, y_n), \quad \alpha = 1/n.$$

Note that the inner product (7) emulates the corresponding inner product in $H^{1,2}([0,1])$. Such emulation is used throughout the theory of Sobolev gradients. The motivating idea is that ϕ does not have an ordinary gradient, at least not one which is continuous and everywhere defined. The gradients $\nabla\phi_n$ have, in a sense, nothing to which to converge. By contrast, the gradients $\nabla_S\phi_n$ converge in an orderly way to the Sobolev gradient of ϕ . The poor numerical performance of ordinary gradients and the good performance of corresponding Sobolev gradients give an instance of the first law of numerical analysis: “Analytical Difficulties and Numerical Difficulties Always Come in Pairs”.

To see a form for the above Sobolev gradient, define

$$D : R^{n+1} \rightarrow R^{2n}$$

so that if $y = (y_0, y_1, \dots, y_n)$, then Dy is the member of R^{2n} whose component k is

$$(y_k + y_{k-1})/2$$

and whose $n+k$ component is

$$(y_k - y_{k-1})/\alpha, \quad k = 1, 2, \dots, n.$$

Problem 5. Show that

$$(\nabla_S\phi_n)(x) = (D^t D)^{-1}(\nabla\phi)_n, \quad x \in R^{n+1}.$$

The above simple example serves as a prototype for creating Sobolev gradients for a wide variety of finite dimensional functionals of interest in numerical approximation of solutions to partial differential equations. Perhaps with the aid of [12] the reader may begin to write code using steepest descent with Sobolev gradients. The following is always the same in cases in which the relevant spaces are inner product spaces: First calculate an ordinary gradient; then the Sobolev gradient is a smoothed (preconditioned) version of this ordinary gradient. The

smoother $(D^t D)^{-1}$ is a positive definite, symmetric matrix which depends on relationship between a Euclidean and a (finite dimensional) Sobolev metric. This relationship ultimately depends on how the Sobolev space in question (here $H^{1,2}([0,1])$) is embedded in the underlying space (here $L_2([0,1])$). Again, see [12] for details.

Problem 6. *An exercise which has often been used to gain insight into Sobolev gradients is the following. Denote $H^{1,2}([0,1]), L_2([0,1])$ by H, K respectively. Here denote by D the differentiation operator on H*

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

Find an expression for D^ , the adjoint of D so that*

$$\langle Df, g \rangle_K = \langle f, D^*g \rangle_H, f \in H, g \in K.$$

What some have found helpful is the use of P , the orthogonal projection of $K \times K$ onto the range of D (see [19]). A solution to this problem is in [12].

Boundary conditions may be incorporated in a Sobolev gradient. This is described in considerable detail in [12]. Here we illustrate this point for our above example. Suppose we wish to enforce the boundary condition $u(0) = 1$ to (6). In this case, We let H_0 be the subspace of H consisting of those members of H which are 0 at 0. Instead of the orthogonal projection P as above, use the orthogonal projection P_0 of $L_2([0,1])^2$ onto

$$\left\{ \begin{pmatrix} y \\ y' \end{pmatrix} : y \in X, y(0) = 1 \right\}.$$

Problem 7. *Construct P_0 .*

A similar consideration holds in the numerical case.

Several applications are now indicated. Related graphical output may be found in [11],[12],[13],[14],[15],[18].

2. GINSBURG-LANDAU FUNCTIONAL AND SUPERCONDUCTIVITY

Suppose that Ω is a bounded region in R^d , for $d = 2$ or 3 . Denote by J the functional on $H = H^{1,2}(\Omega, C) \times H^{1,2}(\Omega, R^n)$ defined by

$$J(u, A) = \int_{\Omega} \|\nabla u\|^2/2 + \|\nabla \times A\|^2/2 + \frac{\kappa^2}{4}(|u|^2 - 1)^2, (u, A) \in H. \quad (8)$$

The function u is called an order parameter, A is called a vector potential. H_0 specifies an imposed magnetic field(it need not be constant on Ω), κ specifies material properties (it also need not be constant: variable κ corresponds to an inhomogeneous material). Once a critical point (u, A) of J is determined, $|u|^2$ gives the density of superconducting electrons; $\nabla \times A$ gives the corresponding induced magnetic field. The corresponding superconducting current can be determined from (u, A) . There is a vast literature on this functional, but we won't attempt to give a guide to this literature here except to mention [17],[4].

We seek numerical critical points of J by means of Sobolev gradients as indicated in Section 1. Results with graphical output have been reported in [13],[15] as well as in [12]. We have observed many critical points of J for various regions Ω , some simply connected and some with various configurations of holes.

A significant problem is the appearance computationally of multiple critical points. There are several questions of interest in this connection:

- Are all apparent critical points actual critical points?
- Are ‘metastable’, i.e., ‘near’ critical points of physical interest?
- If there are multiple critical points, are they of equal scientific interest?
- Is there a preferred selection from among multiple critical points?

Following are some comments on these four questions.

The first questions might be rephrased: Are there metastable critical points? Steepest descent with Sobolev gradients often stays at an energy level for many iterations, only to fall to a lower level (these levels are dictated by number of flux quanta). It seems likely that the answer to the first question is in the negative. Such metastable critical points seem likely to be of physical interest; ‘near’ critical points may indicate superconducting states which last of days as opposed to actual critical points which indicate states lasting for years. A speculation is that if only actual critical points are found (for example solutions to the Euler equations for (8)), then one has the possibility of missing meaningful metastable critical points. It is a challenging problem to articulate workable definitions for metastable states. It seems likely that the answer to the second question is in the affirmative relative to some interesting definition of the term metastable.

Concerning the third question, our experience is that in many circumstances there are multiple critical points, particularly if there are at least two holes in Ω . If a descent computation is started with a simulated vortex situated at one of the holes, it seems to develop into a true vortex pinned to that hole. In short, it appears that the answer to the third question is in the affirmative.

Concerning the fourth question, it seems likely that the answer is in the affirmative. Recently we have developed a code which simulates cooling of a superconducting device. We attempt to describe background for this code and then raise a rather definite mathematical question related to this code. We go into some detail on the last question in the above list.

Given a region Ω of a certain shape, possibly containing holes, and a number $c > 0$ denote by $c\Omega$ the region scaled in linear dimensions by a factor c . Once *fixed*, scaling Ω by a factor c seems of comparable strength to changing κ or H_0 . So if a shape is chosen and one agrees to consider the case of constant κ and H_0 , one essentially has a three parameter system to consider. Many problems of current scientific interest involve choosing parameters c, κ, H_0 so that critical points of the corresponding J have desired properties.

Fix now a bounded region Ω and also fix κ, H_0 . For each $c > 0$ define

$$J_c(u, A) = \int_{c\Omega} \|\nabla u\|^2/2 + \|\nabla \times A - H_c\|^2/2 + \frac{\kappa^2}{4}(|u|^2 - 1)^2, \quad (u, A) \in S_c \quad (9)$$

where S_c denotes the same as H except the relevant spaces are based on $c\Omega$. H_c denotes a scaling of H_0 so that

$$\int_{\Omega} H_0 = \int_{c\Omega} H_c, \quad c \geq 0.$$

Without going in the physics of the situation, we describe the idea back of our recent ‘cooling’ code. Pick an interval $[c_s, c_f]$ of positive numbers. Pick a positive integer k and divide $[c_s, c_f]$ into k pieces of equal length using c_0, c_1, \dots, c_k . Find a critical point of (u_0, A_0) of J_{c_0} . Scale this critical point linearly to the region $c_1\Omega$ and use the up scaled version of (u_0, A_0) to start a steepest descent (always using Sobolev gradients) using J_{c_1} , taking care to scale H_0 to H_{c_1} . Continue this process for $k - 1$ additional steps, at each step scaling the imposed magnetic field so that total magnetic flux is not changed. Question: Is there a limiting value as $k \rightarrow \infty$ and $c_f \rightarrow \infty$, at least if c_s is positive but sufficiently small (for graphical and mathematical purposes keep account of the computation by plotting results on Ω itself using the indicated back scaling). Recent computational (not yet published) points in the direction of this question having an affirmative answer. We realize that the above question leave some latitude in interpretation, particularly that of the relative rates of $k \rightarrow \infty$ and $c_f \rightarrow \infty$, but numerical simulations of the above have been positive. For example if one starts with Ω a rectangular region with a large hole to the left on the horizontal centerline; a smaller hole to the right on the horizontal centerline and a simulated vortex on the horizontal centerline but to the right of the small hole, the computed ‘limiting’ arrangement has been observed to be a vortex captured in the large hole. On a fixed region if one starts with such an initial configuration, the vortex is likely to be captured by the small hole. Somehow the ‘cooling’ process helps the process find the physically most appealing (i.e., the minimal energy one). We are led to believe that actual practice in superconductivity experiments follows this pattern: Start with a device at the end of a rod (say a room temperature), put the rod into a tank of liquid helium (all the time maintaining an imposed magnetic field), then make measurements.

Problem 8. *Formulate and prove a precise conjecture suggested by the above description.*

Problem 9. *A search for critical points of functionals J as in (8) represents an attempt to augment experiments. A well functioning code has the possibility of guiding expensive and time consuming experiments which involve constructing and testing superconducting devices. This is such an important problem that it is certainly desirable having a number of independently written codes that deal with this simulation.*

Problem 10. In [5], for example, there is a description of various Yang-Mills functionals. Someone examining [5] is certain to be struck by the similarity in form of various Yang-Mills functionals and Ginsburg-Landau functionals of superconductivity. The reader is challenged to write a code using Sobolev gradients for some form of the Yang-Mills equations. A main difference between these two problems is that in our present Ginsburg-Landau problems, the order parameter u is complex valued whereas for Yang-Mills, it may be two-by-two unitary matrix valued, for example. Coding for Yang-Mills should not be vastly more difficult than for Ginsburg-Landau for superconductivity.

Problem 11. A final problem in this section deals with the relationship with Sobolev gradient steepest descent with J in (8) and the corresponding time dependent Ginsburg-Landau equations (TDGL), see [16]. In our experience, TDGL evolves states (u, A) in time toward a state of lower energy. Sobolev gradient steepest descent does likewise. It is an appealing thought that somehow these two processes go through quite similar paths. It seems a worthwhile problem to articulate a clear mathematical formulation of this comparison problem. Similar problems occur with other energy functionals.

Problem 12. In [11] there are results on multiple critical points for some energy-like functionals. Can techniques of this reference be used in the case of Ginsburg-Landau functionals?

3. PROBLEMS IN TRANSONIC FLOW

A full potential functional for transonic flow may be expressed as

$$\mathbf{J}(\mathbf{u}) = \int_{\Omega} \left[1 + \frac{\gamma - 1}{2} \|\nabla \mathbf{u}\|^2 \right]^{\gamma/(\gamma-1)}, \quad (10)$$

where Ω is a bounded region in R^d for $d = 1, 2$ or 3 and the domain of J is $H = H^{1,7}(\Omega)$. We make this choice of H since for air, $\gamma = 1.4$. In [12] there are pictures of critical points of such a J in case $d = 2$. It is a fact that there are uncountably many critical points of such a J given appropriate boundary conditions, but generally only one physically viable solution. This situation is clear even in one dimension: Shocks, that is jumps from subsonic to supersonic do not occur in the direction of flow but the opposite kind of jump is observed to occur. Even in one dimension, there are uncountably many critical points which exhibit jumps from subsonic to supersonic in the flow direction, but only one which shows the opposite jump. How to pick out this physically viable critical point? For details we refer to Chapter 13 of [12] which deals with transonic flow, but here indicate that we start by finding a critical point of a functional similar to (10) but containing a rather heavy viscosity term. The viscosity used is considerably more than physically realistic. With this heavy viscosity, no sharp shocks appear. We use this critical point as a starting estimate for a Sobolev gradient descent procedure for a functional similar to (10) but with a lighter viscosity term. After several repetitions of this process we arrive at a critical point which demonstrates sharp shocks which are physically consistent.

The process is similar in spirit to the cooling process described in the previous section.

In [12] there are results of two dimensional runs of flow around a standard airfoil, one ambient subsonic with supersonic shocks above and below the airfoil and one ambient supersonic with a subsonic stagnation pocket in front of the airfoil.

Now (10) requires $H^{1,7}(\Omega)$ for a proper definition. For a C^1 function J from $H^{1,7}(\Omega) \rightarrow R$ and $u \in H^{1,7}(\Omega)$, the Sobolev gradient $(\nabla J)(u)$ is the element $h \in H^{1,7}(\Omega)$ which, following (1), maximizes

$$J'(u)h \text{ subject to } \|h\|_H^{1,7}(\Omega) = |J'(u)|.$$

See [20] and [12] for computational details.

Problem 13. *Code a three dimensional version of (10). In computational fluid dynamics, there are many instances of ‘shock fitting’ (computational intervention in places where exceptional effects are anticipated) vs. ‘shock capturing’ (start with a grid or finite element setting and compute without special intervention). Shock fitting is not so difficult in one dimension; there are many who have learned to do it in two dimensions; few seem to have ambitions for trying it in three dimensions. The pictures for transonic flow in [12] were done using only shock capture and hence it might be suspected that the method has good prospects for three dimensions.*

4. SOME SPECULATION ON BOUNDARY CONDITIONS

The above process shows a feature of Sobolev gradient that has been informally recognized from the start of calculations with Sobolev gradients (in 1976-77 or so but the term ‘Sobolev gradient’ had not been invented yet): Continuous steepest descent (3) with Sobolev gradients (in the presence of boundary conditions which are not sufficient to dictate a single solution) tends to converge to the nearest solution in the appropriate Sobolev metric. As indicated in [12] this is proved for linear problems but in nonlinear problems this remains at the observational level. It is suspected that at least for continuous steepest descent with Sobolev gradients, a convergent process converges to the nearest solution in some yet to be articulated sense, perhaps along some sort of geodesic. Chapter 14 of [12] gives a start of a theory of this sense. Briefly, it is shown that under appropriate hypothesis, if continuous steepest descent converges for every starting value in a function space, then equivalence classes (two starting elements are equivalent if the lead via continuous steepest descent to the same solution) give a way to tag solutions. One hopes to eventually understand sufficiently for significant problems corresponding foliations into equivalence classes in order to provide a solution to the problem of the presentation of all solutions to a given PDE system on a given region. This remains one of the most challenging problems in all of mathematics. In the spirit of the present volume, this challenge is offered to the reader. Following are some specific problems to solution to which might give ideas for a theory on the subject.

Problem 14. Suppose $H = H^{2,2}(\Omega)$ where $\Omega = [0, 1] \times [-1, 1]$ and $F : H \rightarrow K = L_2(\Omega)$ is defined by

$$(F(u))(x, y) = yu_{11}(x, y) + u_{22}(x, y), \quad (x, y) \in \Omega.$$

Define $\phi : H \rightarrow R$ by

$$\phi(u) = \frac{1}{2} \int_{\Omega} F(u)^2, \quad u \in H.$$

Find a useful characterization of

$$Q = \{u \in H : \text{if } z(0) = u, z \text{ satisfies (3), then } \lim_{t \rightarrow \infty} z(t) = 0\}.$$

Observe that Q^\perp is the set of all zeros of F , that is the set of all solutions $u \in H$ to the Tricomi equation

$$yu_{11}(x, y) + u_{22}(x, y) = 0, \quad (x, y) \in \Omega. \quad (11)$$

It seems that despite considerable effort, boundary conditions for have never been articulated (see [9] for a recent reference on Tricomi's equation). The question is raised as to whether some other mechanism than boundary conditions is in order to specify the set of all solutions. In the present linear problem,

$$H \setminus Q$$

is a foliation of H , each member of which contains exactly one solution to (11). A sufficient understanding of this foliation might lead to the comprehension of the set of all solutions to (11). Computations with Sobolev gradients as outlined in the introduction should serve as a laboratory for the understanding of (11). See Chapter 14 of [12] for more discussion on this matter.

Problem 15. Write a Sobolev gradient code for (11). Try to discern properties common to all members of a given equivalence class.

Problem 16. For this problem, suppose that $\Omega = [0, 1]^2$ and $H = C^1(\Omega)$. Consider Burger's equation (without viscosity) on Ω : Find all members $u \in H$ such that

$$u_1 + uu_2 = 0. \quad (12)$$

Observe that if $u \in H$ satisfies (12), then Ω may be filled with intervals so that u is constant on each of these intervals and that moreover, the slope of each interval is that constant value. Reflect on the difficulties of determining the set of all solutions in H to (12) by specifying boundary conditions on some portion of the boundary of Ω . Now define

$$F(u) = u_1 + uu_2, \quad u \in H^{1,2}(\Omega)$$

and define ϕ in terms of F as in the previous problem. Construct a Sobolev gradient for ϕ , both for the function space $H^{1,2}(\Omega)$ and for finite difference approximations. Use resulting numerics to gain insight on how limiting values of (3) correspond to initial estimates. Try to characterize the set of all solutions on Ω to this version of Burger's equation.

This computational problem was the first PDE problem done by the first author (around 1976-77).

Problem 17. *Find a new paradigm to replace boundary conditions in the study of PDE.*

5. MINIMAL SURFACES AND VARIABLE METRICS

Suppose that $\Omega = [0, 1]^2$ and $H = H^{1,2}(\Omega, R^3)$. Denote by H_0 those members of H which are zero on the boundary of Ω . Define $\phi : H \rightarrow R$ so that if $u_1 \times u_2 \neq 0$ on all of Ω , then

$$\phi(u) = \int_{\Omega} \|u_1 \times u_2\|, \quad u \in H,$$

the area function for members of H . Taking a Fréchet derivative,

$$(\phi'(u))h = \int_{\Omega} \langle u_1 \times h_2 + h_1 \times u_2, u_1 \times u_2 \rangle / \|u_1 \times u_2\|, \quad u \in H, h \in H_0.$$

For u as above, consider the following inner product on H_0 :

$$\langle h, k \rangle_u = \int_{\Omega} \langle u_1 \times h_2 + h_1 \times u_2, u_1 \times k_2 + k_1 \times u_2 \rangle / \|u_1 \times u_2\|, \quad h \in H_0. \quad (13)$$

Representing the functional $\phi'(u)$ in the inner product (13), we define a Sobolev gradient by means of the defining relationship

$$(\phi'(u))h = \langle h, (\nabla\phi)(u) \rangle_u.$$

This gives us something like a Hilbert manifold: For each u as above, we attach inner products to the tangent spaces at each element of H . For each $u \in H$ a Sobolev gradient of ϕ at u is defined. As the descent process runs, the metric constantly changes; this is an example of a variable metric where at each step, the metric is adapted to the current estimate.

For $u \in H$ and $\|u_1 \times u_2\|$ bounded away from 0 on Ω define the norm:

$$\|w\|_{L_{2,u}}^2 = \int_{\Omega} \|w\|^2 \|u_1 \times u_2\|, \quad w \in H_0.$$

For this fixed u and for $w \in L_{2,u}$, consider the linear functional $T : H_0 \rightarrow R$ defined by

$$T_w z = \int_{\Omega} z w \|u_1 \times u_2\|, \quad z \in H_0.$$

The transformation T is also continuous with respect to the norm $\|\cdot\|_{L_{2,u}}$ and so it may be represented in the corresponding inner product;

$$T_w z = \langle z, Mw \rangle_u, \quad z \in H_0.$$

The indicated transformation M is the inverse of the laplacian associated with the pair $L_{2,u}, H_0$ (see [12], Chapter 5, [2]). A finite dimensional version of such a transformation M is used as a basis for computation in [14]. Such an M is a surface based laplacian which is distinct from the Laplace-Beltrami operator

acting on functions on the range of u . Much remains to be worked out about such transformations M .

Problem 18. *Make a systematic study of transformations M and the corresponding laplacian M^{-1} .*

6. AN ELASTICITY PROBLEM

Suppose $H = H^{1,2}(\Omega, R^2)$, $\Omega = [0, 1]^2$ and

$$\phi(u, v) = \int_{\Omega} E(u, v)^4 - E(u, v)^2 + \|(\nabla E)(u, v)\|^2 + \frac{1}{2}(F(u, v)^2 + G(u, v)^2), (u, v) \in H.$$

(interpret $(u(x), v(x))$ as displacement at $x \in \Omega$) where

- $2 * E(u, v) = u_1 + v_2$, (deviatoric strain)
- $2 * F(u, v) = u_1 - v_2$, (compression strain)
- $2 * G(u, v) = u_2 + v_1$, (shear strain)

For boundary conditions take $v = 0$ on $\partial\Omega$, $u = 0$, bottom, right, u linear, top, left. In [18] critical points of a numerical version of this function are found.

7. AN OIL-WATER SEPARATION PROBLEM

Take $\Omega = [0, 1]^2$, $H = H^{1,2}(\Omega, R^2)$

$$\phi(u) = \int_{\Omega} \left[\frac{\alpha}{4}(1 - u^2) - Tu + \frac{T}{2}((1 + u) \ln(1 + u) + (1 - u) \ln(1 - u)) + \frac{\kappa}{2}(\|\nabla u\|^2) \right]$$

for $u \in H$. For boundary conditions take

$$u = 0 \text{ top, left, } u = 0.5 \text{ bottom, } u = -0.5 \text{ right.}$$

The non-local condition

$$\int_{\Omega} u = 0.2$$

is also imposed. Sobolev gradients frequently can be made to accommodate such conditions. This is work in progress by the authors of [18]. Excellent identification of oil-water boundary has been obtained without any special computational devices.

8. MORGE-AMPERE PROBLEMS

For this section denote $[0, 1]^2$ by Ω . Suppose $g \in L_2(\Omega)$ is given. Take $H = H^{1,2}(\Omega)$ and denote by H_0 those members of H which are zero on $\partial\Omega$. Consider the problem of finding $u \in H$ so that

$$F(z) = g, z \in H_0. \tag{14}$$

where

$$F(z) = z_{11}z_{22} - z_{12}z_{21}, u \in H.$$

Define $Q : H^{1,2}(\Omega)^2 \rightarrow L_2(\Omega)$ by

$$Q(u, v) = u_1v_2 - u_2v_1, u, v \in H^{1,2}(\Omega).$$

Reformulate (14) as the problem of finding $(u, v) \in H^{1,2}(\Omega)^2$ so that $u = 0$ on the top and bottom of Ω , $v = 0$ on the left and right of Ω and (u, v) is a critical point of ϕ where

$$\phi(u, v) = \frac{1}{2} \int_{\Omega} (Q(u, v) - g)^2, \quad u, v \text{ as above,} \quad (15)$$

and (u, v) are related by the condition $u_2 = v_1$. Consequently z can be obtained from (u, v) by integration.

Problem 19. Write a code to find critical points of a numerical version of (15).

9. CONVERGENCE PROBLEMS

We give here a theorem dealing with convergence of descent processes. A number of others are contained in [12].

Theorem 1. Suppose that H is a Hilbert space, $\Omega \subset H$ and $\phi : H \rightarrow [0, \infty)$ is a C^1 function with locally Lipschitzian derivative. Suppose also that $x \in \Omega$ and $z : [0, \infty) \rightarrow \Omega$ such that

$$z(0) = x, \quad z'(t) = -(\nabla\phi)(z(t)), \quad t \geq 0. \quad (16)$$

Suppose finally that there is $c > 0$, $\theta \in (0, 1)$ so that if $x \in \Omega$,

$$\|(\nabla\phi)(x)\| \geq c\phi(x)^\theta.$$

Then

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

This is a slight generalization of Theorem 4.8 of [12] in which it was required that $\theta = 1/2$. Now (16) is called a Lojasiewicz inequality. In finite dimensional cases, such an inequality is a consequence of analyticity (see [8]) in a neighborhood of a zero of ϕ . An infinite dimensional analogue does not always hold but there are several recent results in which infinite dimensional cases have been proved under additional hypothesis (see [3] for a very recent account of this matter). See also [4] for application of these ideas to Ginsburg-Landau functionals.

Problem 20. Read [3] and attempt to apply ideas to variational problems in this note, in [12], [6] and problems in the present volume.

10. RECOMMENDED READING

In [7] there is an account of the use of Sobolev gradients (Knowles calls Sobolev gradients by another name) in ill-posed problems. This interesting work is related to such problems as numerical differentiation and a number of other topics. This paper is highly recommended as a source of new ideas on the traditionally difficult subject of ill-posed problems.

In [10] there is an account of computational advantages of constructing Sobolev gradients using weighted Sobolev spaces. The interest here is in choosing weights

which are appropriate to singular problems. In a sense, choice of metric for minimal surface problems in this note gives a weighted Sobolev space. These two instances are just the tip of an iceberg on this topic.

It has been a privilege to view a prepublication copy of a new book by Faragó and Karátson [6]. This book contains a great number of interesting problems to which Sobolev gradients apply. The book also contains detailed discussions of these gradients as well as a wealth of information on computations.

REFERENCES

- [1] R.A. Adams, *Sobolev Spaces*, Academic Press, 1978.
- [2] A. Beurling and J. Deny, Dirichlet spaces, Proc. Nat. Acad. Sci. 45 (1959), 208-215.
- [3] R. Chill, *On the Lojasiewicz-Simon Gradient Inequality* (preprint)
- [4] S.-Z. Huang and P. Takač, Convergence in gradient-like systems which are asymptotically autonomous and analytic, Nonlinear Anal. 46 (2001), 675-698.
- [5] A. Jaffe and C. Taubes *Vortices and Monopoles. Structure of Static Gauge Theories*, Progress in Physics 2, 1980.
- [6] I. Faragó and J. Karátson, *Numerical Solution of Nonlinear Elliptic Problems via Preconditioning Operators* (to appear in series *Advances in Computation*, NOVA Science Publishers).
- [7] I. Knowles, *Variational methods for ill-posed problems*, <http://www.math.uab.edu/knowles/pubs.html> .
- [8] S. Lojasiewicz, Une propriété topologique des sous-ensembles analytiques réels, Colloques internationaux du C.N.R.S.: Les équations aux dérivées partielles, Editions du C.N.R.S., Paris (1963), 87-89.
- [9] D. Lupo and K.R. Payne, *On the maximum principle for generalized solutions to the Tricomi problem*, Commun. Contemp. Math. 2 (2000), 535-557.
- [10] W. T. Mahavier, *A convergence result for discrete steepest descent in weighted Sobolev spaces*, Abstract Appl. Anal. (to appear).
- [11] John M. Neuberger, *A numerical method for finding sign-changing solutions of superlinear Dirichlet problems*, Nonlinear World 4 (1997), 73-83.
- [12] J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Springer Lecture Notes in Mathematics 1670, 1997.
- [13] R. J. Renka and J. W. Neuberger *Critical points of the Ginsburg-Landau functional on multiply connected domains*, J. Experimental Mathematics 9 (2000)
- [14] R. J. Renka and J. W. Neuberger *Minimal surfaces and Sobolev gradients*, Siam J. Sci. Comp. 16 (1995), 1412-1427.
- [15] R. J. Renka and J. W. Neuberger, *Sobolev gradients and the Ginsburg-Landau equations*, Siam J. Sci. Comp. 20 (1998), 582-590.
- [16] A. Ardelea, G. F. Carey, A. Pardhanani and W. B. Richardson, *Simulation of Macroscopic Superconductivity for Microelectronics*, Physica C: Superconductivity, V. 341-348, Part 4, (2000), 2649-2650.
- [17] J. Rubinstein, *Six lectures on superconductivity. Interfaces and Transitions.*, CRM Proc. Lec. Notes 13, Amer. Math. Soc., 1998.
- [18] S. Sial, J. Neuberger, T. Lookman, A. Saxena, *Energy minimization using Sobolev gradients: applications to phase separation and ordering.* (submitted for publication).
- [19] J. von Neumann, *Functional Operators II*, Annls. Math. Stud. 22, (1940).
- [20] M. Zahran, *Steepest descent on a uniformly convex space*, Rocky Mountain J. Math (to appear).