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Numerical approximation of time evolution related to Ginzburg–Landau functionals using weighted Sobolev gradients

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ABSTRACT

Sobolev gradients have been discussed in Sial et al. (2003) as a method for energy minimization related to Ginzburg–Landau functionals. In this article, a weighted Sobolev gradient approach for the time evolution of a Ginzburg–Landau functional is presented for different values of κ. A comparison is given between the weighted and unweighted Sobolev gradients in a finite element setting. It is seen that for small values of κ, the weighted Sobolev gradient method becomes more and more efficient compared to using the unweighted Sobolev gradient. A comparison with Newton's method is given where the failure of Newton's method is demonstrated for a test problem.

1. Introduction

Nonlinear phenomena are of fundamental importance in various fields of science and engineering. Nonlinear problems are difficult to solve either analytically or numerically. Many numerical algorithms have been developed for the solution of nonlinear boundary value problems. Weighted Sobolev gradients have been used to treat linear and nonlinear singular differential equations [1]. By careful consideration of the weighting, much improvement can be achieved. The inability of the Newton's method to converge in some situations where the Sobolev gradient approach works has been shown.

For the solution of partial differential equations (PDEs), Sobolev gradient methods [2] have been used in finite-difference [1] and finite-element settings [3]. Sobolev gradients have been successfully applied to physics [4–10], image processing [11,12], geometric modeling [13], material sciences [14–19] and Differential Algebraic Equations (DAEs) [20].

A detailed discussion of Sobolev gradient can be found in [2]. This reference contains existence and sufficient conditions for convergence of the solution. For some applications and open problems in this field we refer the reader to [21].

Computational work was done on an Intel(R) 3 GHz Core(TM)2 Duo machine with 1 GB RAM. We used the open sources FreeFem++ [22] software for the solution of PDEs. All the graphs are drawn using gnuplot software.

2. Sobolev gradient approach

In this section we discuss the Sobolev gradient and steepest descent. A detailed analysis regarding the construction of Sobolev gradients can be seen in [2].

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Suppose that n is a positive integer, F is a real valued C^1 function on R^n. Then the gradient ∇F is defined as

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

For F 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 $\nabla_s F : R^n \to R^n$ so that

$$F'(x)h = \langle h, \nabla_S F(x)\rangle_S \quad x, h \in R^n. \tag{2}$$

The linear functional $F'(x)$ can be represented using any inner product on R^n. Say that $\nabla_S F$ is the gradient of F with respect to the inner product $\langle\cdot,\cdot\rangle_S$ and note that $\nabla_S F$ has the same properties as ∇F.

By taking a linear transformation:

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

these two inner products can be related

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

for $x, y \in R^n$, and a reflection leads to

$$\nabla_S F(x) = A^{-1}\nabla F(x), \quad x \in R^n. \tag{3}$$

Each $x \in R^n$ corresponds to an inner product

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

on R^n. Thus for $x \in R^n$, define $\nabla_x F : R^n \to R^n$ so that

$$F'(x)h = \langle h, \nabla_x F(x)\rangle_x \quad x, h \in R^n. \tag{4}$$

Depending upon the choice of metric, we have a variety of gradients for a function F and these gradients have vastly different numerical properties.

A gradient of a function F is said to be a Sobolev gradient when it is defined in finite or infinite dimensional Sobolev space. Readers who are unfamiliar with Sobolev spaces are referred to [23].

The method of steepest descent is an optimization technique which can be classified into two types: discrete steepest descent and continuous steepest descent.

Let F be a real-valued C^1 function on a Hilbert space H and $\nabla_S F$ be its gradient with respect to the inner product $\langle\cdot,\cdot\rangle_S$ defined on H. Discrete steepest descent denotes, a process of constructing a sequence $\{x_k\}$ such that x_0 is given and

$$x_k = x_{k-1} - \delta_k(\nabla F)(x_{k-1}), \quad k = 1, 2, \ldots \tag{5}$$

where for each k, δ_k is chosen so that it minimizes, if possible,

$$F(x_{k-1} - \delta_k(\nabla F)(x_{k-1})). \tag{6}$$

In continuous steepest descent, we construct a function $z : [0,\infty) \to H$ so that

$$\frac{dz}{dt} = -\nabla F(z(t)), \quad z(0) = z_{\text{initial}}, \tag{7}$$

under suitable conditions on F, $z(t) \to z_\infty$ where $F(z_\infty)$ is the minimum value of F.

Continuous steepest descent is interpreted as a limiting case of discrete steepest descent and so (5) can be considered as a numerical method for approximating solutions to (7). Continuous steepest descent provides a theoretical starting point for proving convergence for discrete steepest descent.

Using (5) one seeks $u = \lim_{k\to\infty} x_k$, so that

$$F(u) = 0 \quad \text{or} \quad (\nabla_S F)(u) = 0. \tag{8}$$

Using (7), one seeks $u = \lim_{t\to\infty} z_t$ so that (8) holds.

To solve a partial differential equation (PDE), we construct F by a variational principle, i.e., there is a function F and we have a function u that satisfies the differential equation if and only if u is a critical point of F. In these situations we try to use a steepest descent minimization process to find a zero of the gradient of F.

In our case

$$F(u) = \int_\Omega \delta_t\frac{u^4}{4} + (1-\delta_t)\frac{u^2}{2} - fu + \delta_t\frac{\kappa}{2}|\nabla u|^2. \tag{9}$$

Note that other functionals are also possible and one of the prime examples in this direction is least square formulation. Such functions are shown in [9,16]. In this paper, we only shows results from which F comes by a variational principle as the results in this setting are optimal [16].

The existence and convergence of $z(t) \to z(\infty)$ for different linear and nonlinear forms of F is discussed in [2].