Weighted Sobolev Descent for Singular First Order Partial Differential Equations

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Abstract

The author's work on solving singular ordinary differential equations via steepest descent based on weighted Sobolev gradients is extended to first order partial differential equations with linear singularities. Results are presented which demonstrate the improvements obtained by computing based on weighted Sobolev gradients.

1 Introduction

A general discussion of optimization techniques is given in [9] and [15]. Applying steepest descent to solve differential equations was first introduced by Cauchy in [2] and modifications such as conjugate gradient and variable metric methods, [6], were later introduced to speed up the convergence of numerical implementations. Sobolev descent is a systematic preconditioning technique where gradients are based on Sobolev spaces determined by the problem at hand rather than on Euclidean space. The method was introduced by J. W. Neuberger in [13] along with sufficient conditions for convergence and a complete discussion of Soblev descent may be found in [14]. The extension of the technique to singular ordinary differential equations by utilizing weighted Sobolev spaces based on the problem at hand, [11], compliments and extends his work. In [10] a convergence proof is given for discrete spaces such as those in this paper. Existence and uniqueness arguments for singular problems in Sobolev spaces are given in [18] and [3]. For a paper concerning Sobolev gradients which are constructed based on the problem at hand, consider [16]. Problem specific applications of Sobolev descent are given in, [4], [5], [7], [12] and [17]. General references for Sobolev spaces are [1] and [8].

2 Preliminaries

Let $I = [0,1]$, $\Omega \subset \Re^2$, and $L = \left(L^2_\Omega, \langle\cdot,\cdot\rangle_L\right)$. Define $\pi_1,\ \pi_2 : \Re\times\Re \to \Re$ by $\pi_1\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \alpha$ and $\pi_2\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \beta$. Suppose $a, b \in C^1_\Omega$ vanish at only finitely many points in Ω, $u \in C^1_\Omega$, and $\vec{v} = (v_1, v_2)$ is a vector valued function on $\Re^2$. We make the following definitions:

$$\begin{array}{l}
\nabla u = (u_x, u_y) = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)\\
\nabla\cdot\vec{v} = (v_1)_x + (v_2)_y\\
\nabla_w u = (au_x, bu_y)\\
\nabla_w\cdot\vec{v} = a(v_1)_x + b(v_2)_y\\
\Delta u = \nabla^2 u = \nabla\cdot\nabla u = u_{xx} + u_{yy}\\
\Delta_w u = \nabla^2_w u = \nabla_w\cdot\nabla_w u = a(au_x)_x + b(bu_y)_y
\end{array} \tag{1}$$

$$G_w = \overline{\left\{\begin{pmatrix} u\\ \nabla_w u\end{pmatrix} : u \in C^1_\Omega\right\}}^{L\times(L\times L)}.$$

Definition 1 *H_w is the collection of functions which appear as first coordinates of elements of G_w.*

Theorem 1 *If $a, b \in C^1_\Omega$ and a, b vanish at only finitely many points in Ω then G_w is a function.*

Proof. Let $\mathcal{P}$ denote the polynomials on Ω. Suppose $\begin{pmatrix}u\\ v\end{pmatrix}, \begin{pmatrix}u\\ w\end{pmatrix} \in G_w$. The linearity of G_w implies that $\begin{pmatrix}0\\ v-w\end{pmatrix} \in G_w$. Since there exists a sequence, $(u_k)_{k\in\mathbf{N}} \in C^1_\Omega$ such that $\begin{pmatrix}u_k\\ \nabla_w u_k\end{pmatrix} \to \begin{pmatrix}0\\ v-w\end{pmatrix}$, it suffices to show that given $\begin{pmatrix}0\\ \begin{pmatrix}f\\ g\end{pmatrix}\end{pmatrix} \in G_w$, we have $\begin{pmatrix}f\\ g\end{pmatrix} = 0$ in $L\times L$. Let $\begin{pmatrix}f\\ g\end{pmatrix} \in G_w$ and $(u_k)_{k\in\mathbf{N}}$ such that $\begin{pmatrix}u_k\\ \nabla_w u_k\end{pmatrix} \to \begin{pmatrix}0\\ \begin{pmatrix}f\\ g\end{pmatrix}\end{pmatrix}$. Let $p, q \in \mathcal{P}$, $F = \begin{pmatrix}p\\ q\end{pmatrix}$, and $F_w = \begin{pmatrix}ap\\ bq\end{pmatrix}$.

$$\begin{aligned}
\left|\left\langle\begin{pmatrix}f\\ g\end{pmatrix}, \begin{pmatrix}p\\ q\end{pmatrix}\right\rangle_{L\times L}\right| &\le \left|\left\langle\begin{pmatrix}f\\ g\end{pmatrix} - \begin{pmatrix}a(u_k)_x\\ b(u_k)_y\end{pmatrix}, \begin{pmatrix}p\\ q\end{pmatrix}\right\rangle_{L\times L}\right| + \left|\left\langle\begin{pmatrix}a(u_k)_x\\ b(u_k)_y\end{pmatrix}, \begin{pmatrix}p\\ q\end{pmatrix}\right\rangle_{L\times L}\right|\\
&\le \left\|\begin{pmatrix}f\\ g\end{pmatrix} - \begin{pmatrix}a(u_k)_x\\ b(u_k)_y\end{pmatrix}\right\|_{L\times L} \|F\|_L + \left|\int_\Omega \nabla_w u_k\cdot F\right|\\
&= \left\|\begin{pmatrix}f\\ g\end{pmatrix} - \begin{pmatrix}a(u_k)_x\\ b(u_k)_y\end{pmatrix}\right\|_{L\times L} \|F\|_L + \left|\int_\Omega \nabla u_k\cdot F_w\right|
\end{aligned}$$

$$\leq \ \| \begin{pmatrix} f \\ g \end{pmatrix} - \begin{pmatrix} a(u_k)_x \\ b(u_k)_y \end{pmatrix} \|_{L\times L} \ \|F\|_L + |\int_{\partial\Omega} u_k(F_w \cdot N)| + |\int_{\Omega} u_k(\nabla \cdot F_w)|$$
$$\leq \ \| \begin{pmatrix} f \\ g \end{pmatrix} - \begin{pmatrix} a(u_k)_x \\ b(u_k)_y \end{pmatrix} \|_{L\times L} \ \|F\|_L + |\int_{\partial\Omega} u_k(F_w \cdot N)| + \|u_k\|_L \ \|\nabla \cdot F_w\|_L$$

As $k \to \infty$, all three summands tend to zero, from which it follows that $\left\langle \begin{pmatrix} f \\ g \end{pmatrix}, \begin{pmatrix} p \\ q \end{pmatrix} \right\rangle_{L\times L} = 0$ for all $p, q \in \mathcal{P}$, a dense subset of L. *q.e.d.*

Define three operators on H_w by

$$\begin{aligned} E_0(u) &= u \\ E_1^a(u) &= \pi_1 G_w u \\ E_2^b(u) &= \pi_2 G_w u. \end{aligned}$$

Thus, $G_w u = \left(E_1^a u, E_2^b u\right)$ is the generalized weighted gradient. If $u \in C^1_\Omega$ then $G_w u = \nabla_w u$. Define an inner product on H_w by

$$\langle u, v\rangle_{H_w} = \langle u, v\rangle_L + \langle E_1^a(u), E_1^a(v)\rangle_L + \left\langle E_2^b(u), E_2^b(v)\right\rangle_L$$

The case $a \equiv 1 \equiv b$ has been studied, [14]. Without regard to boundary conditions, the spaces under consideration are H and H_w where H represents the unweighted Sobolev space obtained when $a \equiv 1 \equiv b$.

Theorem 2 *G_w is a closed, bounded, non-expansive, densely defined operator on H_w.*

Proof. G_w is closed by definition. Let $\mathcal{P}$ denote the polynomials on Ω. Since, $\mathcal{P}$ is dense in L, and $\mathcal{P} \subset G_w \subset L$, G_w is densely defined. For any $u \in H_w$,

$$\frac{\|G_w u\|_L}{\|u\|_{H_w}} = \frac{\|G_w u\|_L}{\|u\|_L + \|G_w u\|_L} \leq 1,$$

thus G_w is bounded and non-expansive from H_w to L. *q.e.d.*

Theorem 3 *H_w is a Hilbert space.*

Proof. Let $(u_n)_{n\in\mathbf{N}}$ be a Cauchy sequence in H_w. Thus $\begin{pmatrix} u_n \\ G_w u_n \end{pmatrix}_{n\in\mathbf{N}}$ is a Cauchy sequence in G_w which is complete as a closed subspace of the complete space, $L \times L$. Let $\begin{pmatrix} f \\ g \end{pmatrix} \in G_w$ such that $\begin{pmatrix} u_n \\ G_w u_n \end{pmatrix}_{n\in\mathbf{N}} \to \begin{pmatrix} f \\ g \end{pmatrix}$. Now, $(u_n)_{n\in\mathbf{N}} \to f$ in H_w. *q.e.d.*

In order to develop gradients depending on the constraints we define the following spaces dependent upon the boundary conditions.

Definition 2 *Suppose B is a linear operator representing the boundary conditions and put $L^0 = \{u \in L : Bu = 0\}$ and $H_w^0 = H_w \cap L^0$.*

Denote by $\pi_L : L \to L^0$ the orthogonal projection under $\langle \cdot, \cdot \rangle_L$ and denote by $\pi_{H_w} : H_w \to H_w^0$ the orthogonal projection under $\langle \cdot, \cdot \rangle_{H_w}$.

The next definition is used to define gradients based on $L, L^0, H, H^0, H_w, and H_w^0$.

Definition 3 *If S is any Hilbert space, $J : S \to \Re$ is a bounded linear functional, and $s \in S$, define $\nabla_S J(s)$ to be the unique element in S such that $J'(s)(r) = \langle \nabla_s J(s), r \rangle_S$ for all $s \in S$.*

The following theorem, [12], guarantees convergence in the continuous setting. Related convergence results for the discrete case are offered in [9] and [13].

Theorem 4 *(J. W. Neuberger) Suppose $\mathcal{H}$ and $\mathcal{K}$ are Hilbert spaces and $G \in L(\mathcal{H}, \mathcal{K})$. Suppose $g \in \mathcal{K}$, $v \in \mathcal{H}$, $Gv = g$, and $\phi(u) = \frac{1}{2}\|Gu - g\|^2$ for every $u \in \mathcal{H}$. If $x \in \mathcal{H}$ and z is the function on $[0, \infty)$ so that*

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

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

3 An Example

Consider the class of problems,

$$\begin{array}{l} a, b \in C^2_\Omega \\ \Omega = [0,1] \times [0,1] \\ au_x + bu_y = 0 \\ u(x,x) = 2x^2 \ \forall \ x \in [0,1]. \end{array} \tag{2}$$

Define the functional,

$$J(u) = \frac{1}{2} \int_\Omega (au_x + bu_y)^2 \, d\Omega.$$

The gradient on which descent is denoted by $\nabla_{H_w^0} J$ and is the unique element in the Hilbert space H_w^0 which satisfies, $J'(u)(h) = \left\langle \left(\nabla_{H_w^0} J \right)(u), h \right\rangle$ for all $u, h \in H_w^0$ as constructed via Definition 3. For all $u \in H_w, h \in H_w^0$ we have,

$$\begin{array}{rcl} J'(u)(h) & = & \langle \left(\nabla_H J \right)(u), h \rangle \\ & = & \langle \left(\nabla_H J \right)(u), \pi_{H_w} h \rangle \\ & = & \langle \pi_{H_w} \left(\nabla_H J \right)(u), h \rangle \end{array}$$

Hence for all $u, h \in H_w^0$, $\left\langle \left(\nabla_{H_w^0} J \right)(u), h \right\rangle = \langle \pi_{H_w} \left(\nabla_H J \right)(u), h \rangle$ and $\left(\nabla_{H_w^0} J \right)(u) = \pi_{H_w} \left(\nabla_H J \right)(u)$.

For $u \in H_w$ define

$$J(u) = \frac{1}{2}\int_\Omega (E_1^a u + E_2^b u)^2 \, d\Omega.$$

The iteration is now,

$$u^{k+1} = u^k - \delta_k \left(\nabla_{H_w^0} J\right)(u^k)$$

where δ_k is given by the smallest positive real number that minimizes $\alpha(\delta_k) = J\big(u^k - \delta_k \left(\nabla_{H_w} J\right)(u^k)\big)$. Setting $\alpha'(\delta_k) = 0$ and solving yields the optimal step size,

$$\delta_k = \frac{\| \left(\nabla_{H_w} J\right)(u^k)\|_{H_w}^2}{\left\langle \left(\nabla_{H_w} J\right)^2 (u^k), \left(\nabla_{H_w} J\right)(u^k)\right\rangle_{H_w}}.$$

3.1 Numerical Considerations

Subdivide Ω into n pieces along each axis. Order the grid starting in the lower left hand corner at $(0,0)$ so that $u_{i,j} = u(\frac{1}{n}(i-1), \frac{1}{n}(j-1))$.

Discrete versions of u, $E_0(u)$, $E_1^a(u)$, and $E_2^b(u)$ are subscripted as matrices, but are treated as vectors. Their definitions follow:

$$u = \begin{pmatrix} u_{1,1} \\ u_{2,1} \\ \vdots \\ u_{n+1,n+1} \end{pmatrix}, \quad E_0(u) = \begin{pmatrix} \{E_0(u)\}_{1,1} \\ \{E_0(u)\}_{2,1} \\ \vdots \\ \{E_0(u)\}_{n+1,n+1} \end{pmatrix}, \quad E_w(u) = \begin{pmatrix} E_0(u) \\ E_1^a(u) \\ E_2^b(u) \end{pmatrix}.$$

$$\left\{ E_0 \begin{pmatrix} u_{1,1} \\ u_{2,1} \\ \vdots \\ u_{n+1,n+1} \end{pmatrix} \right\}_{i,j} = \frac{1}{4}(u_{i,j} + u_{i+1,j} + u_{i,j+1} + u_{i+1,j+1})$$

$$\left\{ E_1^a \begin{pmatrix} u_{1,1} \\ u_{2,1} \\ \vdots \\ u_{n+1,n+1} \end{pmatrix} \right\}_{i,j} = \frac{n}{4}(a_{i,j} + a_{i+1,j})(-u_{i,j} + u_{i+1,j} - u_{i,j+1} + u_{i+1,j+1})$$

$$\left\{ E_2^b \begin{pmatrix} u_{1,1} \\ u_{2,1} \\ \vdots \\ u_{n+1,n+1} \end{pmatrix} \right\}_{i,j} = \frac{n}{4}(b_{i,j} + b_{i,j+1})(-u_{i,j} - u_{i+1,j} + u_{i,j+1} + u_{i+1,j+1})$$

The discretized versions of the spaces L and H_w are $\left(\Re^{(n+1)^2}, \langle\cdot,\cdot\rangle_L\right)$, and $\left(\Re^{(n+1)^2}, \langle\cdot,\cdot\rangle_{H_w}\right)$ where $\langle\cdot,\cdot\rangle_L$ denotes the Euclidean inner product and $\langle u, v\rangle_{H_w} = \langle E_0 u, E_0 v\rangle_L + \langle E_1^a u, E_1^a v\rangle_L + \left\langle E_2^b u, E_2^b v\right\rangle_L$.

Discretizing our functional yields,

$$\begin{aligned} J(u) &= \frac{1}{2}\int_\Omega (au_x + bu_y)^2\, d\Omega \\ &= \frac{1}{2}\int_\Omega (E_1^a u + E_2^b u)^2\, d\Omega \\ &\cong \frac{1}{2n^2}\sum_{i,j}^{n}(\{E_1^a u\}_{i,j} + \{E_2^b u\}_{i,j})^2 \end{aligned}$$

The discrete analog to $(\nabla_L J)$ is $\nabla J = \begin{pmatrix} \frac{\partial J}{\partial u_{1,1}} \\ \frac{\partial J}{\partial u_{2,1}} \\ \vdots \\ \frac{\partial J}{\partial u_{n+1,n+1}} \end{pmatrix}$. Four summands from our functional, J, contribute to $\frac{\partial J}{\partial u_{p,q}}$.

$$\begin{aligned} \frac{\partial J}{\partial u_{p,q}} &= \frac{1}{2n^2}\frac{\partial}{\partial u_{p,q}}\Bigg\{ \left[(E_1^a u)_{p-1,q-1} + \left(E_2^b u\right)_{p-1,q-1}\right]^2 \\ &\quad + \left[(E_1^a u)_{p,\ q-1} + \left(E_2^b u\right)_{p,\ q-1}\right]^2 \\ &\quad + \left[(E_1^a u)_{p-1,q} + \left(E_2^b u\right)_{p-1,q}\right]^2 \\ &\quad + \left[(E_1^a u)_{p,\ q} + \left(E_2^b u\right)_{p,\ q}\right]^2 \Bigg\} \\ &= \frac{1}{n^2}\Bigg\{ \left[(E_1^a u)_{p-1,q-1} + \left(E_2^b u\right)_{p-1,q-1}\right]\left[\frac{n}{4}\left(a_{p-1,q-1} + a_{p,q-1}\right) + \frac{n}{4}\left(b_{p-1,q-1} + b_{p-1,q}\right)\right] + \\ &\quad \left[(E_1^a u)_{p,\ q-1} + \left(E_2^b u\right)_{p,\ q-1}\right]\left[-\frac{n}{4}\left(a_{p,q-1} + a_{p+1,q-1}\right) + \frac{n}{4}\left(b_{p,q-1} + b_{p,q}\right)\right] + \\ &\quad \left[(E_1^a u)_{p-1,q} + \left(E_2^b u\right)_{p-1,q}\right]\left[\frac{n}{4}\left(a_{p-1,q} + a_{p,q}\right) - \frac{n}{4}\left(b_{p-1,q} + b_{p-1,q+1}\right)\right] + \\ &\quad \left[(E_1^a u)_{p-1,q} + \left(E_2^b u\right)_{p-1,q}\right]\left[-\frac{n}{4}\left(a_{p,q} + a_{p+1,q}\right) - \frac{n}{4}\left(b_{p,q} + b_{p,q+1}\right)\right] \Bigg\} \end{aligned}$$

The two inner products are related by, $\langle u, v\rangle_{H_w} = \langle Au, v\rangle_L$ where $A = (E_0)^t E_0 + (E_1^a)^t E_1^a + (E_2^b)^t E_2^b$.

The canonical perturbation space will be $\Re_0^{(n+1)^2} = \left\{x \in \Re^{(n+1)^2} | Bx = 0\right\}$ where B is the linear operator representing our boundary conditions. Let π_{H_w} :

$\Re^{(n+1)^2} \to \Re_0^{(n+1)^2}$ denote the orthogonal projection under $\langle \cdot,\cdot \rangle_{H_w}$ and $\pi_L : \Re^{(n+1)^2} \to \Re_0^{(n+1)^2}$ denote the orthogonal projection under $\langle \cdot,\cdot \rangle_{L.}$

Applying the Reisz Representation Theorem twice and using the self-adjoint property of projections repeatedly we have for every $u \in \Re^{(n+1)^2}, h \in \Re_0^{(n+1)^2}$,

$$\begin{aligned}
\langle \pi_L(\nabla J)(u), h\rangle_L &= \langle (\nabla J)(u), \pi_L h\rangle_L \\
&= \langle (\nabla J)(u), h\rangle_L \\
&= J'(u)(h) \\
&= \langle \left(\nabla_{H_w} J\right)(u), h\rangle_{H_w} \\
&= \langle \left(\nabla_{H_w} J\right)(u), \pi_{H_w} h\rangle_{H_w} \\
&= \langle \pi_{H_w}\left(\nabla_{H_w} J\right)(u), h\rangle_{H_w} \\
&= \left\langle \left(\nabla_{H_w^0} J\right)(u), h\right\rangle_{H_w} \\
&= \left\langle A\left(\nabla_{H_w^0} J\right)(u), h\right\rangle_L \\
&= \left\langle A\left(\nabla_{H_w^0} J\right)(u), \pi_L h\right\rangle_L \\
&= \left\langle \pi_L A\left(\nabla_{H_w^0} J\right)(u), h\right\rangle_L
\end{aligned}$$

Consequently, $\pi_L A\left(\nabla_{H_w^0} J\right)(u) = \pi_L\left(\nabla_L J\right)(u)$ is valid for every $u \in \Re^{(n+1)^2}$ and provides a linear system allowing us to solve for $\left(\nabla_{H_w^0} J\right)(u)$.

Solving for $x_{i,j} = \left\{\left(\nabla_{H_w^0} J\right)(u)\right\}_{i,j}$ indicates that $x_{i,j}$ receives contributions from eight of the nine non-zero bands of A that correspond to the eight "neighbors" of $x_{i,j}$, $(i.e. x_{i-1,j-1}, x_{i-1,j}, ..., x_{i+1,j+1})$. We solve the system via SOR.

3.2 Results

The results in this section are for the equation,

$$\begin{array}{l} yu_x - xu_y = 0 \\ u(x,x) = 2x^2 \ \forall \ x \in I \end{array} \tag{3}$$

which has solution $u(x,y) = x^2 + y^2$. Tables 1 and 2 demonstrate two features of the algorithm. First observe the significant improvements in the obtainable accuracy by utilizing the weighted steepest descent. Second observe that the results in Table 1 are based on a 10 x 10 grid and yet are representative of the results (except for run time) in Table 2 which are based on a 50 x 50 grid.

The three rows represent descent based on the Eucliden, the non-weighted and the weighted gradients respectively. The three columns represent the divided difference error, the average absolute error, and the maximum absolute error. If u represents the computed solution, then the divided difference error is given by,

$$\sum_{i,j}^{n} |\{E_1^a u\}_{i,j} + \{E_2^b u\}_{i,j}|/(n+1)^2,$$

Table 1: Singular Partial Differential Equation

$\mathbf{yu_1 - xu_2 = 0}$		$\mathbf{u(x,x) = 2x^2}$		$\mathbf{Grid = 10 \times 10}$	
Gradient	Iterations	Seconds	Div. Dif. Err.	Avg. Abs. Err.	Max. Abs. Err.
L	$3,031$	$0:10$	10^{-5}	10^{-4}	7.1×10^{-4}
H	$1,315$	$0:18$	10^{-5}	10^{-4}	6.6×10^{-4}
H_w	25	$0:1$	10^{-4}	10^{-4}	4.2×10^{-4}

Table 2: Singular Partial Differential Equation

$\mathbf{yu_1 - xu_2 = 0}$		$\mathbf{u(x,x) = 2x^2}$		$\mathbf{Grid = 50 \times 50}$	
Gradient	Iterations	Min:Sec	Div. Dif. Err.	Avg. Abs. Err.	Max. Abs. Err.
L	$46,282$	$62:20$	10^{-5}	10^{-4}	2.1×10^{-3}
H	$1,334$	$10:23$	10^{-4}	10^{-4}	2.1×10^{-3}
H_w	25	$5:04$	10^{-4}	10^{-5}	7.6×10^{-4}

while the average absolute error is given by,

$$\sum_{i,j}^{n} |u_{i,j} - 2\frac{1}{n}(i-1)\frac{1}{n}(j-1)|/(n+1)^2.$$

4 Conclusions

The algorithm gives good results on a small number of divisions making the algorithm a candidate for multi-grid methods.

Improvements to the algorithm as presented would be to incorporate multi-grid techniques, appropriate SOR constants, and conjugate gradient technology.

A “C” code for the algorithm may be obtained from the author along with a Mathematica code for computation of the matrices involved.

Preliminary investigations indicate that the method extends to second order equations such as:

$$\begin{array}{l} f(u) = \lambda u + u^3 \\ \Omega = Cl(B[0,1]) \\ \Delta u + f(u) = 0 \\ u|_{\partial\Omega} = 0. \end{array} \tag{4}$$

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