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THE BEST WEIGHTED GRADIENT APPROXIMATION TO AN OBSERVED FUNCTION

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Abstract

We find the potential function whose gradient best approximates an observed square integrable function on a bounded open set subject to prescribed weight factors. With an appropriate choice of topology, we show that the gradient operator is a bounded linear operator and that the desired potential function is obtained by solving a second-order, self-adjoint, linear, elliptic partial differential equation. The main result makes a precise analogy with a standard procedure for the best approximate solution of a system of linear algebraic equations. The use of bounded operators means that the definitive equation is expressed in terms of well-defined functions and that the error in a numerical solution can be calculated by direct substitution into this equation. The proposed method is illustrated with a hypothetical example.

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1. Introduction

Let $\boldsymbol{x}$ denote the general position vector in $\mathbb{R}^3$ and let Ω be a nonempty bounded open set in $\mathbb{R}^3$ with piecewise-smooth boundary $\partial\Omega$. Suppose that an observed square integrable function $\boldsymbol{f} : \Omega \to \mathbb{C}^3$ is given. We wish to find the potential function $u : \Omega \to \mathbb{C}$ with $u(\boldsymbol{x}) = 0$ when $\boldsymbol{x} \in \partial\Omega$, which minimises the total weighted residual error

$$\int_\Omega \|R(\boldsymbol{x})(\boldsymbol{\nabla} u(\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}))\|^2 \, dV(\boldsymbol{x}),$$

where $R : \Omega \to \mathbb{C}^{3\times 3}$ is an infinitely differentiable, nonsingular weight function and $dV(\boldsymbol{x})$ is the differential volume element in Ω.

1.1. Main contribution. We make an analogy between the solution of linear algebraic equations and the solution of linear differential equations.

In linear algebra it is well known that the matrix equation $A\boldsymbol{x} = \boldsymbol{b}$, where $A \in \mathbb{C}^{m\times n}$ and $\boldsymbol{b} \in \mathbb{C}^m$, may have no solution $\boldsymbol{x} \in \mathbb{C}^n$. In such circumstances it is routine to seek the best approximate solution. Thus, one seeks a vector $\boldsymbol{x}_0 \in \mathbb{C}^n$ which minimises the mean-square error $\|A\boldsymbol{x} - \boldsymbol{b}\|$ over all $\boldsymbol{x} \in \mathbb{C}^n$. The vector $\boldsymbol{x}_0$ can be found by solving the equation

$$A^* A\boldsymbol{x} = A^*\boldsymbol{b}. \tag{1.1}$$

Equation (1.1) is guaranteed to have a solution and the solution is unique if the self-adjoint matrix $A^*A \in \mathbb{C}^{n\times n}$ is strictly positive. It is standard practice to represent the best approximate solution $\boldsymbol{x}_0$ as a series using the orthogonal eigenvectors of A^*A as a basis for $\mathbb{C}^n$.

It is not so well known generally that a similar approach can be followed with linear differential equations. Thus, the prime purpose of this paper is to show—albeit on the basis of some well-established and fundamental analysis—that the complex-valued first-order differential equation $\boldsymbol{\nabla} u = \boldsymbol{f}$, where $\boldsymbol{f} : \Omega \to \mathbb{C}^3$ for some bounded open set $\Omega \subset \mathbb{R}^3$ with $u(\boldsymbol{x}) = 0$ when $\boldsymbol{x} \in \partial\Omega$, can be treated in an exactly analogous way. It is certainly true that the gradient equation may not have an exact solution. Consider, for instance, the case where $\boldsymbol{\nabla} \times \boldsymbol{f} \neq \boldsymbol{0}$. However, if the problem is formulated for a function $u : \Omega \to \mathbb{C}$ in an appropriate Sobolev space—the Hilbert space $H_0 = H_0^1(\Omega)$ of complex-valued functions with a square integrable generalised gradient—then the gradient operator $T \in \mathcal{L}(H_0, K)$ defined by $Tu = \boldsymbol{\nabla} u$ for all $u \in H_0$ is a bounded linear map from H_0 into the space $K = L^2(\Omega)^3$ of square integrable complex vector-valued functions. The best approximate solution to the gradient equation $Tu = \boldsymbol{f}$, where $\boldsymbol{f} \in K$, can be found by using the projection theorem to find the function $u_0 \in H_0$ that minimises the mean-square error $\|Tu - \boldsymbol{f}\|_K$. Furthermore, we can find the unique solution u_0 by solving the self-adjoint elliptic differential equation

$$T^*Tu = T^*\boldsymbol{f}.$$

An implicit observation—our subliminal message—is that the iconic second-order elliptic differential equations of mathematical physics arise as a simple consequence of our desire to solve a basic gradient approximation problem. We will relate our proposed methodology to the classical analysis of elliptic differential equations where the gradient operator $S : H_0 \subset G \to K$ defined by $Su = \boldsymbol{\nabla} u$ for $u \in H_0$ is regarded as a densely defined unbounded operator on the space $G = L^2(\Omega)$ of square integrable complex-valued functions. This has important implications because the compactness of $(S^*S)^{-1} \in \mathcal{L}(G)$ can be used to show that the spectrum of $(T^*T)^{-1} = (S^*S)^{-1}(I + S^*S) \in \mathcal{L}(H_0)$ is discrete. Thus, we find an explicit series form for our solution $u_0 \in H_0$ using the orthogonal eigenvectors of $(T^*T)^{-1}$ as a basis for H_0.

1.2. Previous work. The technique of finding a best approximate solution to an inconsistent system of linear algebraic equations is well known. The same principles apply to the solution of inconsistent linear differential equations but the analogy with linear algebraic equations is seldom drawn. It is certainly true that the relevant mathematical techniques are known and well used in the solution of self-adjoint, linear, elliptic differential equations. However, the idea that elliptic differential equations arise as a consequence of gradient approximation—the best approximate solution to an inconsistent first-order partial differential equation—has apparently not been widely canvassed. For this reason the works we cite are primarily expositions of the underlying classical analysis developed during the first half of the twentieth century. A general background to this analysis can be found in Aubin [1], Kinderlehrer and Stampacchia [3], Luenberger [4], Naylor and Sell [5], Treves [6], Yosida [7] and Ziedler [8]. We refer specifically to the relevant fundamental theory in these texts. We have used spaces of complex-valued functions throughout for two reasons. In the first instance much of the classical work on self-adjoint differential operators in our main references [5, 7, 8] is formulated in this way. In the second instance the Fourier transform—a popular tool in computational work—is often expressed in terms of complex-valued functions. The results in this paper extend those given in [2] in the following ways. In the original paper the region of interest was the unit cube and there were no weight functions used in the various inner products. Consequently, the relevant second-order self-adjoint differential equation is the basic Poisson equation on the unit cube. This equation has an explicit solution in closed form. In this paper the region of interest is a general bounded open set with piecewise-smooth boundary and the inner products involve arbitrary smooth weight functions. The necessary existence and uniqueness theory—which we outline in some detail—for the corresponding second-order self-adjoint differential equation is mathematically more general and more challenging.

1.3. Organisation of the paper. The remainder of the paper is organised as follows. In Section 2 we outline the underlying functional analysis. This section also contains specific definitions that are needed to explain the main result. We pay particular attention to formulation of the gradient operator as a bounded linear operator $T \in \mathcal{L}(H_0^1(\Omega), L^2(\Omega))$ and to derivation of a formula for the corresponding adjoint operator $T^* \in \mathcal{L}(L^2(\Omega), H_0^1(\Omega))$. In Section 3 we review the theoretical basis for solution of second-order elliptic partial differential equations by considering a weighted Poisson equation. Our motivation here is to relate the classical formulation using unbounded differential operators to an equivalent formulation using bounded operators. The main result concerning gradient approximation is stated precisely and proved in Section 4. We conclude our discussion in Section 5 by considering a hypothetical example.

2. Preliminary notes

We need to establish our terminology and some basic functional analysis.

2.1. The basic function spaces. Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with piecewise-smooth boundary $\partial\Omega$. The linear space $C^\infty(\Omega)$ is the space of all complex-valued functions $\varphi : \Omega \to \mathbb{C}$ with continuous partial derivatives of all orders. The space $C_0^\infty(\Omega)$ is the subspace of all such functions φ with compact support $\mathrm{spt}(\varphi) \subset \Omega$.

Let $p \in C^\infty(\Omega)$ be an infinitely differentiable, real-valued weight function which satisfies the inequalities $\delta \le p(\boldsymbol{x}) \le D$ for some real numbers $0 < \delta \le D$ and all $\boldsymbol{x} \in \Omega$. The space $G = L^2(\Omega)$ is the set of all complex-valued measurable functions $u : \Omega \to \mathbb{C}$

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such that

$$\int_{\Omega} |u(x)|^2 \, dV(\boldsymbol{x}) < \infty$$

with inner product

$$\langle u, v\rangle_G = \int_{\Omega} u(\boldsymbol{x})v(\boldsymbol{x})p(\boldsymbol{x}) \, dV(\boldsymbol{x}). \tag{2.1}$$

The inner product (2.1) is topologically equivalent to the usual inner product [7, page 40] because of the bounds on p. The elements of $C_0^\infty(\Omega)$ form a dense subset in G. That is, for each $u \in G$, we can find $\{\varphi_m\}_{m\in\mathbb{N}} \in C_0^\infty(\Omega)$ with $\|\varphi_m - u\|_G \to 0$ as $m \to \infty$.

There are two related function spaces that will be used throughout our discussion. We will assume that the known, infinitely differentiable, complex-valued matrix weight function $R \in C^\infty(\Omega)^{3\times 3}$ satisfies the property

$$\epsilon \|\boldsymbol{b}\|^2 \le \|R(\boldsymbol{x})\boldsymbol{b}\|^2 \le E\|\boldsymbol{b}\|^2 \tag{2.2}$$

for some given real numbers $0 < \epsilon \le E$ and for any $\boldsymbol{b} \in \mathbb{C}^3$ and all $\boldsymbol{x} \in \Omega$. Define the Hilbert space $H = H^1(\Omega)$ of complex-valued measurable functions $u : \Omega \mapsto \mathbb{C}$ with measurable generalised gradients such that

$$\int_{\Omega} [|u(\boldsymbol{x})|^2 + \|\boldsymbol{\nabla} u(\boldsymbol{x})\|^2] \, dV(\boldsymbol{x}) < \infty$$

and with inner product

$$\langle u, v\rangle_H = \int_{\Omega} [u(\boldsymbol{x})\overline{v(\boldsymbol{x})}p(\boldsymbol{x}) + \langle R(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x}), R(\boldsymbol{x})\boldsymbol{\nabla} v(\boldsymbol{x})\rangle] \, dV(\boldsymbol{x}) \tag{2.3}$$

for each $u, v \in H$. We use the notation $\langle \boldsymbol{b}, \boldsymbol{c}\rangle = b_1\overline{c_1} + b_2\overline{c_2} + b_3\overline{c_3}$ to denote the inner product in the complex Euclidean space $\mathbb{C}^3$ with $\|\boldsymbol{b}\| = \langle \boldsymbol{b}, \boldsymbol{b}\rangle^{1/2}$ for the associated norm. Since R is bounded by (2.2), the inner product (2.3) is topologically equivalent to the usual inner product [7, pages 57–59]. We write $H_0 = H_0^1(\Omega)$ for the subspace of H with $u(\boldsymbol{x}) = 0$ when $\boldsymbol{x} \in \partial\Omega$. The space $C_0^\infty(\Omega)$ forms a dense subspace of H_0. That is, for each $u \in H_0$, we can find $\{\varphi_m\}_{m\in\mathbb{N}} \in C_0^\infty(\Omega)$ with $\|\varphi_m - u\|_H \to 0$ as $m \to \infty$. Note also that H_0 can be regarded as a subspace of G. Let $K = L^2(\Omega)^3$ denote the Hilbert space of square integrable functions $\boldsymbol{k} : \Omega \mapsto \mathbb{C}^3$ such that

$$\int_{\Omega} \|\boldsymbol{k}(\boldsymbol{x})\|^2 \, dV(\boldsymbol{x}) < \infty$$

with inner product

$$\langle \boldsymbol{k}, \boldsymbol{\ell}\rangle_K = \int_{\Omega} \langle R(\boldsymbol{x})\boldsymbol{k}(\boldsymbol{x}), R(\boldsymbol{x})\boldsymbol{\ell}(\boldsymbol{x})\rangle \, dV(\boldsymbol{x}) \tag{2.4}$$

for each $\boldsymbol{k}, \boldsymbol{\ell} \in K$. The space $C^\infty(\Omega)^3$ forms a dense subspace of K. That is, for each $\boldsymbol{f} \in K$, we can find $\{\boldsymbol{\psi}_m\}_{m\in\mathbb{N}} \in C^\infty(\Omega)^3$ such that $\|\boldsymbol{\psi}_m - \boldsymbol{f}\|_K \to 0$ as $m \to \infty$.

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2.2. The bounded gradient operator. The mapping $T : H_0 \mapsto K$ defined by $Tu = \boldsymbol{\nabla} u$, where

$$\boldsymbol{\nabla} u = \begin{bmatrix} \dfrac{\partial u}{\partial x_1} \\ \dfrac{\partial u}{\partial x_2} \\ \dfrac{\partial u}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \partial_1 u \\ \partial_2 u \\ \partial_3 u \end{bmatrix},$$

is a bounded linear map. We call T the bounded gradient operator. The adjoint map $T^* \in \mathcal{L}(K, H_0)$ is also a bounded linear map given by $T^*\boldsymbol{f} = v_f$, where $v_f \in H_0$ is the uniquely defined function with

$$\langle u, v_f\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K$$

for all $u \in H_0$. It is useful to outline the general argument. Let $\boldsymbol{f} \in K$. The operator $L_f \in \mathcal{L}(H_0, \mathbb{C})$ defined by $L_f(u) = \langle Tu, \boldsymbol{f}\rangle_K$ is a bounded linear operator. Define the subspace $N_f = \{u \in H_0 \mid \langle Tu, \boldsymbol{f}\rangle_K = 0\} \subset H_0$. If $N_f = H_0$, then we set $T^*\boldsymbol{f} = v_f = 0$ and we have $\langle u, v_f\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K = 0$ for all $u \in H_0$. If $N_f \neq H_0$, then we choose $w_f \in N_f^\perp$ with $w_f \neq 0$. We must have $\langle Tw_f, \boldsymbol{f}\rangle_K = c_f \neq 0$. Define a bounded linear map $A \in \mathcal{L}(H_0)$ by the formula

$$A(u) = u - (1/c_f)\langle Tu, \boldsymbol{f}\rangle_K w_f.$$

Since $\langle TA(u), \boldsymbol{f}\rangle_K = 0$, it follows that $A(u) \in N_f$. Hence,

$$\langle A(u), w_f\rangle_H = 0 \iff \langle u, c_f w_f/\|w_f\|_H^2\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K$$

for all $u \in H_0$. Thus, we set $T^*\boldsymbol{f} = v_f = c_f w_f/\|w_f\|_H^2$ and we have $\langle u, v_f\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K$ for all $u \in H_0$. For more information, see Luenberger [4, pages 109–110 and 150–157].

2.3. The bounded adjoint gradient operator. Our next task is to establish the important formula

$$T^*\boldsymbol{f} = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle,$$

where $W = R^*R$, for all $\boldsymbol{f} \in K$. To do this, we must digress for a moment to define the generalised weighted divergence operator, which we write in the form $\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle$.

2.3.1. The generalised weighted divergence. Since Ω is bounded, it follows that $C_0^\infty(\Omega) \subset H_0$. For each $\theta \in C^\infty(\Omega)$, we define a corresponding linear functional $L_\theta : C_0^\infty(\Omega) \to \mathbb{C}$ by the formula

$$L_\theta(\varphi) = \langle \varphi, (1/p)\theta\rangle_G = \int_\Omega \varphi(\boldsymbol{x})\overline{\theta(\boldsymbol{x})}\, dV(\boldsymbol{x}).$$

We shall use this definition as the basis for a number of key ideas. Let $W \in C^\infty(\Omega)^3$ be the continuously differentiable, self-adjoint, strictly positive matrix-valued function defined by $W(\boldsymbol{x}) = R^*(\boldsymbol{x})R(\boldsymbol{x})$ for all $\boldsymbol{x} \in \Omega$.

Lemma 2.1. *Let $\boldsymbol{\psi} \in C^\infty(\Omega)^3$. For all $\varphi \in C_0^\infty(\Omega)$,*

$$\langle \varphi, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\psi}\rangle\rangle_G = (-1)\langle \boldsymbol{\nabla}\varphi, \boldsymbol{\psi}\rangle_K.$$

Proof. For convenience, let $\boldsymbol{\omega} = W\boldsymbol{\psi}$. Write

$$\langle \boldsymbol{\nabla}, \boldsymbol{\omega}\rangle = \frac{\partial \omega_1}{\partial x_1} + \frac{\partial \omega_2}{\partial x_2} + \frac{\partial \omega_3}{\partial x_3} = \partial_1\omega_1 + \partial_2\omega_2 + \partial_3\omega_3$$

to denote the divergence of $\boldsymbol{\omega} \in C^\infty(\Omega)^3$. It is conventional to write the divergence of the vector-valued function $\boldsymbol{\omega} = \boldsymbol{\omega}(\boldsymbol{x}) \in \mathbb{R}^3$ in the form $\boldsymbol{\nabla} \cdot \boldsymbol{\omega}$ in deference to a superficial resemblance to the scalar product $\boldsymbol{p} \cdot \boldsymbol{q}$ for $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^3$. Here, however, we write $\langle \boldsymbol{b}, \boldsymbol{c}\rangle$ for the scalar product of $\boldsymbol{b}, \boldsymbol{c} \in \mathbb{C}^3$ and so for $\boldsymbol{\omega} = \boldsymbol{\omega}(\boldsymbol{x}) \in \mathbb{C}^3$ we prefer to write the divergence as $\langle \boldsymbol{\nabla}, \boldsymbol{\omega}\rangle$ despite some deficiencies in the analogy. By the product rule of differentiation,

$$\langle \boldsymbol{\nabla}, \varphi(\boldsymbol{x})\overline{\boldsymbol{\omega}(\boldsymbol{x})}\rangle = \langle \boldsymbol{\nabla}\varphi(\boldsymbol{x}), \boldsymbol{\omega}(\boldsymbol{x})\rangle + \varphi(\boldsymbol{x})\overline{\langle \boldsymbol{\nabla}, \boldsymbol{\omega}(\boldsymbol{x})\rangle}$$

for each $\boldsymbol{x} \in \Omega$ and so

$$\begin{aligned}\int_\Omega \langle \boldsymbol{\nabla}, \varphi(\boldsymbol{x})\overline{\boldsymbol{\omega}(\boldsymbol{x})}\rangle \, dV(\boldsymbol{x}) &= \int_\Omega [\langle \boldsymbol{\nabla}\varphi(\boldsymbol{x}), \boldsymbol{\omega}(\boldsymbol{x})\rangle + \varphi(\boldsymbol{x})\overline{\langle \boldsymbol{\nabla}, \boldsymbol{\omega}(\boldsymbol{x})\rangle}] \, dV(\boldsymbol{x}) \\ &= \int_\Omega [\langle \boldsymbol{\nabla}\varphi(\boldsymbol{x}), W(\boldsymbol{x})\boldsymbol{\psi}(\boldsymbol{x})\rangle + \varphi(\boldsymbol{x})\overline{\langle \boldsymbol{\nabla}, W(\boldsymbol{x})\boldsymbol{\psi}(\boldsymbol{x})\rangle}] \, dV(\boldsymbol{x}) \\ &= \langle \boldsymbol{\nabla}\varphi, \boldsymbol{\psi}\rangle_K + \langle \varphi, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\psi}\rangle\rangle_G.\end{aligned}$$

Let $\boldsymbol{n}(\boldsymbol{x})$ denote the unit outward normal to the surface $\partial\Omega$ at the point $\boldsymbol{x}$. Since $\varphi(\boldsymbol{x}) = 0$ for $\boldsymbol{x} \in \partial\Omega$, it follows from the Gauss–Ostrogradsky divergence theorem that

$$\int_\Omega \langle \boldsymbol{\nabla}, \varphi(\boldsymbol{x})\overline{\boldsymbol{\omega}(\boldsymbol{x})}\rangle \, dV(\boldsymbol{x}) = \int_{\partial\Omega} \langle \varphi(\boldsymbol{x})\overline{\boldsymbol{\omega}(\boldsymbol{x})}, \boldsymbol{n}(\boldsymbol{x})\rangle \, dS(\boldsymbol{x}) = 0,$$

where $dS(\boldsymbol{x})$ denotes the differential element of surface area. This establishes the desired result. □

Definition 2.2. For each $\boldsymbol{f} \in K$, we define the generalised weighted divergence operator $L_{(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle} : C_0^\infty(\Omega) \mapsto \mathbb{C}$ by the formula

$$L_{(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(\varphi) = \langle \varphi, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle\rangle_G = (-1)\langle \boldsymbol{\nabla}\varphi, \boldsymbol{f}\rangle_K. \tag{2.5}$$

Remark 2.3. Equation (2.5) shows that $L_{(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle}$ is a linear functional on $C_0^\infty(\Omega)$. If $\{\boldsymbol{\psi}_m\}_{m\in\mathbb{N}} \in C^\infty(\Omega)^3$ with $\|\boldsymbol{\psi}_m - \boldsymbol{f}\|_K \to 0$ as $m \to \infty$, then

$$\langle \varphi, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\psi}_m\rangle\rangle_G = (-1)\langle \boldsymbol{\nabla}\varphi, \boldsymbol{\psi}_m\rangle_K \to (-1)\langle \boldsymbol{\nabla}\varphi, \boldsymbol{f}\rangle_K$$

as $m \to \infty$ for all $\varphi \in C_0^\infty(\Omega)$.

Definition 2.4. For each $\boldsymbol{f} \in K$, the generalised weighted divergence operator can be extended to a bounded linear functional $L_{(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle} \in \mathcal{L}(H_0, \mathbb{C})$ using the formula

$$L_{(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(u) = \langle u, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle\rangle_G = (-1)\langle \boldsymbol{\nabla}u, \boldsymbol{f}\rangle_K$$

for all $u \in H_0$.

REMARK 2.5. Choose $\{\varphi_m\}_{m\in\mathbb{N}} \in C_0^\infty(\Omega)$ so that $\|\varphi_m - u\|_H \to 0$ as $m \to \infty$. Now it can be seen that

$$|\langle \varphi_m - \varphi_n, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle\rangle_G| = |\langle \boldsymbol{\nabla}(\varphi_m - \varphi_n), \boldsymbol{f}\rangle_K| \\ \leq \|\boldsymbol{\nabla}(\varphi_m - \varphi_n)\|_K \|\boldsymbol{f}\|_K \to 0$$

as $m, n \to \infty$ because $\|\boldsymbol{\nabla}(\varphi_m - \varphi_n)\|_K \leq \|\varphi_m - \varphi_n\|_H \to 0$. Therefore, there exists $L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(u) \in \mathbb{C}$ such that $L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(\varphi_m) \to L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(u)$ as $m \to \infty$. Clearly,

$$|L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle}(u)| = |(-1)\langle \boldsymbol{\nabla} u, \boldsymbol{f}\rangle_K| \leq \|\boldsymbol{\nabla} u\|_K \|\boldsymbol{f}\|_K \leq \|\boldsymbol{f}\|_K \|u\|_H$$

and so $L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle} \in \mathcal{L}(H_0, \mathbb{C})$ with $\|L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{f}\rangle}\| \leq \|\boldsymbol{f}\|_K$.

When $\theta \in C_0^\infty(\Omega)$, we write $\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle\theta = \langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\theta\rangle = \sum_{i,j=1}^3 \partial_i[w_{ij}\partial_j\theta]$ to emphasise the linear dependence on θ. Let $u, v \in H_0$ and choose a sequence $\{\varphi_m\}_{m\in\mathbb{N}} \in C_0^\infty(\Omega)$ with $\|\varphi_m - u\|_H \to 0$ as $m \to \infty$ and a sequence $\{\theta_n\}_{n\in\mathbb{N}} \in C_0^\infty(\Omega)$ with $\|\theta_n - v\|_H \to 0$ as $n \to \infty$. Since

$$\langle \varphi_m, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle\theta_n\rangle_G = (-1)\langle \boldsymbol{\nabla}\varphi_m, \boldsymbol{\nabla}\theta_n\rangle_K$$

for all $m, n \in \mathbb{N}$, we may take the limit as $m, n \to \infty$ to obtain

$$\langle u, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle v\rangle_G = (-1)\langle \boldsymbol{\nabla} u, \boldsymbol{\nabla} v\rangle_K. \tag{2.6}$$

By interchanging the roles of u, v in Equation (2.6) and taking the complex conjugate,

$$\langle u, (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle v\rangle_G = \langle (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u, v\rangle_G$$

for all $u, v \in H_0$. Since H_0 is dense in G, it follows that the unbounded linear mapping $L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle} : H_0 \subset G \to G$ is self adjoint on G. Finally

$$\langle (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u, u\rangle_G = (-1)\|\boldsymbol{\nabla} u\|_K^2 < 0$$

for all $u \in H_0$ and so the mapping $L_{(1/p)\langle\boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle}$ is *dissipative*. See [7, page 208].

2.3.2. Derivation of the key adjoint formula. Now suppose $\boldsymbol{f} \in K$ and let $T^*\boldsymbol{f} = v \in H_0$ be the uniquely defined element such that

$$\langle u, v\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K \tag{2.7}$$

for all $u \in H_0$. Equation (2.7) can be expressed in integral form as

$$\int_\Omega [u(\boldsymbol{x})\overline{v(\boldsymbol{x})}p(\boldsymbol{x}) + \langle R(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x}), R(\boldsymbol{x})\boldsymbol{\nabla} v(\boldsymbol{x})\rangle]\, dV(\boldsymbol{x}) \\ = (-1)\int_\Omega u(\boldsymbol{x})\overline{\langle \boldsymbol{\nabla}, W(\boldsymbol{x})\boldsymbol{f}(\boldsymbol{x})\rangle}\, dV(\boldsymbol{x})$$

and then rewritten in terms of the generalised weighted divergence as

$$\langle u, (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)v\rangle_G = \langle u, (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle\rangle_G$$

for all $u \in H_0$. Since $v = T^* \boldsymbol{f}$, we have established that

$$(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)T^* \boldsymbol{f} = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle \tag{2.8}$$

for all $\boldsymbol{f} \in K$. Now we note that

$$\langle u, (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)v\rangle_G = \langle u, v\rangle_G + \langle \boldsymbol{\nabla} u, \boldsymbol{\nabla} v\rangle_K = \langle u, v\rangle_H$$

for all $u, v \in H_0$ and hence

$$\langle u, (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)u\rangle_G = \|u\|_H^2 > 0$$

for all $u \in H_0$. Therefore, the strictly positive, unbounded linear operator $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle) : H_0 \subset G \to G$ satisfies a standard Gårding inequality

$$\langle u, (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)u\rangle_G \geq \|u\|_H^2. \tag{2.9}$$

For an extended discussion of Gårding inequalities in this context, see Naylor and Sell [5, pages 505–509]. See also Yosida [7, pages 175–182]. By Rellich's theorem [5, pages 506–508], we know that $(H_0, \|\cdot\|_H)$ is compact in $(G, \|\cdot\|_G)$ and hence by [5, Theorem 7.6.4, pages 508–509] it follows that $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1} \in \mathcal{L}(G)$ is a well-defined compact linear operator. Since $\|u\|_H \geq \|u\|_G$, it is apparent from Equation (2.9) that $\|(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)\| \geq 1$. Thus, $\|(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}\| \leq 1$. Now we can express Equation (2.8) in the equivalent form

$$T^* \boldsymbol{f} = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle \tag{2.10}$$

for all $\boldsymbol{f} \in K$. If $\boldsymbol{f} = Tv$ for some $v \in H_0$, then formula (2.10) becomes

$$T^* T v = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle v$$

for all $v \in H_0$. We shall call $(-1)T^*T \in \mathcal{L}(H_0)$ the bounded weighted Laplacian operator.

2.3.3. Calculating the bounded adjoint gradient operator. The operator $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle) : H_0 \subset G \to G$ is an unbounded, self-adjoint operator on G with a compact inverse $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1} \in \mathcal{L}(G)$. Therefore, there exist a countable collection of real, nonnegative eigenvalues $\{\lambda_m\}_{m\in\mathbb{N}}$ for $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)$ and a corresponding collection $\{u_m\}_{m\in\mathbb{N}} \in G$ of orthogonal eigenfunctions which form a basis for G. Since

$$\langle (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)u_m, u_n\rangle_G = \langle u_m, u_n\rangle_H \Longrightarrow \lambda_m\langle u_m, u_n\rangle_G = \langle u_m, u_n\rangle_H,$$

we see that $\{u_m\}_{m\in\mathbb{N}}$ is also orthogonal in H_0 with $\lambda_m = \|u_m\|_H^2/\|u_m\|_G^2 > 1$ for all $m \in \mathbb{N}$. Note that by [3, Corollary A.11, pages 57–58], there is some constant $C = C(\Omega) > 0$ with $\|u\|_G \leq C\|\boldsymbol{\nabla} u\|_K$ for all $u \in H_0$ and hence it is not possible to have $\|u\|_H = \|u\|_G$ for $u \neq 0$. We will write $\lambda_m = \sigma_m^2 + 1$ and order the eigenvalues so that $0 < \sigma_m \leq \sigma_{m+1}$ for all $m \in \mathbb{N}$. Since the eigenvalues of $(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}$ are given by the nonincreasing sequence $\{1/\lambda_m\}_{m\in\mathbb{N}}$ and since the only possible limit point is 0, we have $0 \leq 1/\lambda_m \leq 1/\lambda_1 < 1$. Therefore,

$$\langle u, (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)u\rangle_G \geq \lambda_1\|u\|_H^2. \tag{2.11}$$

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We will normalise the eigenvectors to make $\{u_m\}_{m\in\mathbb{N}}$ an orthonormal basis for H_0. For each $u \in H_0$,

$$u = \sum_{m=1}^{\infty} \langle u, u_m\rangle_H u_m$$

and so we calculate $T^*Tu = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u$ as

$$T^*Tu = \sum_{m=1}^{\infty} \frac{\langle u, u_m\rangle_H \sigma_m^2}{\sigma_m^2 + 1} u_m. \tag{2.12}$$

Since

$$\sum_{m=1}^{\infty} |\langle u, u_m\rangle_H|^2 \sigma_m^4/(\sigma_m^2+1)^2 < \sum_{n=1}^{\infty} |\langle u, u_m\rangle_H|^2 = \|u\|_H^2 < \infty,$$

we see that the series (2.12) converges to a well-defined element of H_0. Now suppose $\boldsymbol{f} \in K$. Since $T \in \mathcal{L}(H_0)$ is a bounded linear operator, it follows that $T(H_0)$ is a closed subspace of K. Hence, we can write $\boldsymbol{f} = Tu_f + \boldsymbol{r} = \boldsymbol{\nabla} u_f + \boldsymbol{r}$, where $u_f \in H_0$ and $\langle \boldsymbol{\nabla} u, \boldsymbol{r}\rangle_K = 0$ for all $u \in H_0$. From $\langle \boldsymbol{\nabla}, W\boldsymbol{r}\rangle(\varphi) = \langle \boldsymbol{\nabla}\varphi, \boldsymbol{r}\rangle_K = 0$ for all $\varphi \in C_0^\infty(\Omega)$, we have $\langle \boldsymbol{\nabla}, W\boldsymbol{r}\rangle = 0$. Therefore,

$$\begin{aligned} T^*\boldsymbol{f} &= (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W(\boldsymbol{\nabla} u_f + \boldsymbol{r})\rangle \\ &= (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u_f \\ &= T^*Tu_f. \end{aligned}$$

We use the basis $\{u_m\}_{m\in\mathbb{N}}$ for H_0 to construct a corresponding orthonormal basis $\{\boldsymbol{w}_m\}_{m\in\mathbb{N}}$ for $T(H_0)$ by setting $\boldsymbol{w}_m = (\sqrt{\sigma_m^2+1}/\sigma_m)\boldsymbol{\nabla} u_m$ for all $m \in \mathbb{N}$. It follows that

$$\begin{aligned} Tu_f &= \sum_{m=1}^{\infty} \langle \boldsymbol{\nabla} u_f, \boldsymbol{w}_m\rangle_K \boldsymbol{w}_m \\ &= \sum_{m=1}^{\infty} \langle \boldsymbol{f}, \boldsymbol{w}_m\rangle_K \Big(\sqrt{\sigma_m^2+1}/\sigma_m\Big) Tu_m. \end{aligned}$$

Therefore, $T^*\boldsymbol{f} = T^*Tu_f \in H_0$ is an ordinary function defined by

$$\begin{aligned} T^*\boldsymbol{f} &= \sum_{m=1}^{\infty} \langle \boldsymbol{f}, \boldsymbol{w}_m\rangle_K \Big(\sqrt{\sigma_m^2+1}/\sigma_m\Big) T^*Tu_m \\ &= \sum_{m=1}^{\infty} \frac{\langle \boldsymbol{f}, \boldsymbol{w}_m\rangle_K\, \sigma_m}{\sqrt{\sigma_m^2+1}} u_m. \end{aligned} \tag{2.13}$$

The operator $T^*T \in \mathcal{L}(H_0)$ is defined by the formula

$$T^*Tu = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u$$

for all $u \in H_0$. We note that $\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle u$ may be a generalised function. However, we can rearrange the terms to obtain

$$T^*Tu = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}u$$

for all $u \in H_0$. Thus, we can now calculate $w = (I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}u \in H_0$ and then $z = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle w \in H_0$. The same rearrangement can be used to calculate $T^*\boldsymbol{f} = T^*Tu_f$.

3. Elliptic differential operators

The study of elliptic partial differential operators was initially motivated by consideration of fundamental problems in the physical sciences. For instance, the electrostatic potential $\varphi(\boldsymbol{x})$ in some bounded domain $\Omega \subset \mathbb{R}^3$ in free space due to a known charge density distribution $\rho(\boldsymbol{x})$ is determined as the solution to the Poisson equation

$$(-1)\nabla^2\varphi = (1/\varepsilon_0)\rho,$$

where ε_0 is the permittivity of free space. The operator $\nabla^2 = \langle \boldsymbol{\nabla}, \boldsymbol{\nabla}\rangle$ is called the Laplacian differential operator. The Poisson equation is an archetypal form of the famous Dirichlet problem—the historical origin for the theory of elliptic partial differential equations. We will consider the unbounded elliptic differential operator $L : H_0 \subset G \to G$ given by

$$\begin{aligned} Lu(\boldsymbol{x}) &= (-1)(1/p(\boldsymbol{x}))\langle \boldsymbol{\nabla}, W(\boldsymbol{x})\boldsymbol{\nabla}\rangle u(\boldsymbol{x}) \\ &= (-1)(1/p(\boldsymbol{x}))\sum_{i=1}^{3}\sum_{j=1}^{3}\partial_i[w_{ij}(\boldsymbol{x})\partial_j]u(\boldsymbol{x}) \end{aligned}$$

for each $u \in H_0$ and the associated weighted Poisson equation

$$Lu = w, \tag{3.1}$$

where $w \in H_0$ is given. If there exists a real constant $\epsilon > 0$ such that $\langle \boldsymbol{b}, W(\boldsymbol{x})\boldsymbol{b}\rangle = \|R(\boldsymbol{x})\boldsymbol{b}\|^2 > \epsilon\|\boldsymbol{b}\|^2$ for all $\boldsymbol{x} \in \Omega$, then the operator L is strongly elliptic [7, page 176]. Now it follows by [5, Corollary 7.8.4 and subsequent discussion on page 520] that L satisfies a Gårding inequality in the form $\langle \varphi, L\varphi\rangle_G \geq c_1\|\varphi\|_H^2$ for some real constant $c_1 > 0$. In fact, since $I + L = I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle$, the Gårding inequality follows from Equation (2.11) with $c_1 = \lambda_1 - 1 = \sigma_1^2$. Now Rellich's theorem [5, pages 506–508] shows that $(H_0, \|\cdot\|_H)$ is compact in $(G, \|\cdot\|_G)$ and so we can see by [5, Theorem 7.6.4, pages 508–509] that $L^{-1} \in \mathcal{L}(G)$ exists and is compact with $L^{-1}(G) \subset H_0$. Therefore, Equation (3.1) has a solution $u_0 \in H_0$. This solution is essentially a classical solution. For more information, see Yosida [7, pages 177–182] and Naylor and Sell [5, pages 516–520].

As we saw in the previous paragraph, the traditional approach to solution of elliptic differential equations treats the operator $L : H_0 \subset G \to G$ as a densely defined, unbounded operator. This approach is fundamental to our understanding of self-adjoint elliptic differential operators because it implies that the inverse operator $L^{-1} \in \mathcal{L}(G)$ is compact. Hence, L^{-1} has a countable collection of real, positive eigenvalues. Therefore, we can represent the solution to Equation (3.1) as a series of orthogonal functions.

We will now relate the traditional unbounded elliptic differential operators to the corresponding bounded operators used in the solution of our gradient approximation problem. The unbounded linear operator $S : H_0 \subset G \to K$ is defined by the formula $Su = \boldsymbol{\nabla} u$ and, hence, by Lemma 2.1,

$$\langle S\varphi, \boldsymbol{\psi}\rangle_K = (-1)\langle \varphi, (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\psi}\rangle\rangle_G$$

for all $\varphi \in C_0^\infty(\Omega)$ and $\boldsymbol{\psi} \in C^\infty(\Omega)^3$. By taking appropriate limits, and arguing as we did earlier in the paper,

$$S^*\boldsymbol{f} = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle$$

for all $\boldsymbol{f} \in H_0^3 \subset K$. Now it is instructive to consider the relationship between the bounded adjoint gradient mapping $T^* : K \to H_0$ and the unbounded adjoint gradient mapping $S^* : H_0^3 \subset K \to G$. We have

$$\langle u, T^*\boldsymbol{f}\rangle_H = \langle Tu, \boldsymbol{f}\rangle_K = \langle Su, \boldsymbol{f}\rangle_K = \langle u, S^*\boldsymbol{f}\rangle_G$$

and

$$\begin{aligned}\langle u, T^*\boldsymbol{f}\rangle_H &= \langle u, T^*\boldsymbol{f}\rangle_G + \langle Su, ST^*\boldsymbol{f}\rangle_K\\ &= \langle u, T^*\boldsymbol{f}\rangle_G + \langle u, S^*ST^*\boldsymbol{f}\rangle_G\\ &= \langle u, (I + S^*S)T^*\boldsymbol{f}\rangle_G.\end{aligned}$$

So, by combining the two previous equations,

$$\langle u, S^*\boldsymbol{f}\rangle_G = \langle u, (I + S^*S)T^*\boldsymbol{f}\rangle_G$$

for all $u \in H_0$ and all $\boldsymbol{f} \in H_0^3$. A mild extension of an important result due to von Neumann [7, page 200] states that for a densely defined, closed unbounded linear operator $S : H_0 \subset G \mapsto K$ there exist well-defined inverse operators $(I + S^*S)^{-1} \in \mathcal{L}(G)$ and $(I + SS^*)^{-1} \in \mathcal{L}(K)$. Hence,

$$(I + S^*S)T^*\boldsymbol{\psi} = S^*\boldsymbol{\psi} \iff T^*\boldsymbol{\psi} = (I + S^*S)^{-1}S^*\boldsymbol{\psi} = S^*(I + SS^*)^{-1}\boldsymbol{\psi}$$

for all $\boldsymbol{\psi} \in C_0^\infty(\Omega)$. Since $\|T^*\| \le 1$, it follows that for $\boldsymbol{f} \in K$ and any sequence $\{\boldsymbol{\psi}_m\}_{m\in\mathbb{N}} \in C^\infty(\Omega)$ with $\|\boldsymbol{\psi}_m - \boldsymbol{f}\| \to 0$, we have $\|\boldsymbol{\psi}_m - \boldsymbol{\psi}_n\|_K \to 0$ as $m, n \to \infty$ and hence $\|T^*\boldsymbol{\psi}_m - T^*\boldsymbol{\psi}_n\|_H \to 0$ as $m, n \to \infty$. Thus, we can find $v_f \in H_0$ such that $T^*\boldsymbol{\psi}_n \to v_f$ and so $T^*\boldsymbol{f} = v_f$ can be rewritten as $S^*(I + SS^*)^{-1}\boldsymbol{f} = v_f$. Now $P = T^*T = (I + S^*S)^{-1}S^*S = S^*S(I + S^*S)^{-1} \in \mathcal{L}(H_0)$ and $Q = TT^* = (I + SS^*)^{-1}SS^* = SS^*(I + SS^*)^{-1} \in \mathcal{L}(K)$ are both self adjoint. Note also that $L = S^*S$ and that

$$T^*T = (I + S^*S)^{-1}S^*S = I - (I + S^*S)^{-1} \iff (I + S^*S)^{-1} = I - T^*T.$$

It follows that

$$Lu = w \iff S^*Su = w \iff T^*Tu = (I - T^*T)w$$

and hence

$$u = L^{-1}w \iff u = (S^*S)^{-1}w \iff u = (T^*T)^{-1}(I - T^*T)w.$$

Thus, we can describe the weighted Poisson equation and the solution using either unbounded or bounded linear differential operators.

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4. The best weighted gradient approximation

We state the solution to the general weighted gradient approximation as our main theorem.

THEOREM 4.1. *Let $\boldsymbol{f} \in K$ be an observed function and let $T \in \mathcal{L}(H_0, K)$ be the bounded gradient operator. The solution to the weighted gradient approximation problem*

$$\inf_{u \in H_0} \|Tu - \boldsymbol{f}\|_K$$

is defined as the unique function $u_0 \in H_0$ satisfying the self-adjoint differential equation $T^*Tu = T^*\boldsymbol{f}$. If the inner products on H_0 and K are defined by (2.3) and (2.4), respectively, then the equation $T^*Tu = T^*\boldsymbol{f}$ can be written in the expanded form as

$$\begin{aligned}(-1)(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}&(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}u\rangle \\ &= (-1)(I - (1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}\rangle)^{-1}(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle. \qquad (4.1)\end{aligned}$$

Let $\{u_m\}_{m\in\mathbb{N}}$ be an orthonormal basis of eigenvectors for T^*T in H_0 with $T^*Tu_m = \sigma_m^2/(\sigma_m^2 + 1)u_m$ and define a corresponding orthonormal set $\{\boldsymbol{w}_m\}_{m\in\mathbb{N}}$ in K by the formula $\boldsymbol{w}_m = (\sqrt{\sigma_m^2 + 1}/\sigma_m)\boldsymbol{\nabla}u_m$. If we define the projection of $\boldsymbol{f}$ onto the subspace spanned by $\{\boldsymbol{w}_m\}_{m\in\mathbb{N}}$ using the formula $\boldsymbol{w}_f = \sum_{m=1}^{\infty}\langle \boldsymbol{f}, \boldsymbol{w}_m\rangle_K \boldsymbol{w}_m$, then the solution to the best weighted gradient approximation problem is given by

$$u_0 = \sum_{m=1}^{\infty}\langle \boldsymbol{f}, \boldsymbol{w}_m\rangle_K\Big(\sqrt{\sigma_m^2 + 1}/\sigma_m\Big)u_m \qquad (4.2)$$

for all $\boldsymbol{f} \in K$.

PROOF. Since $T(H_0) \subset K$ is a closed subspace, we can use the projection theorem to find a point $Tu_0 \in T(H_0)$ such that $\langle Tu_0 - \boldsymbol{f}, Tu\rangle_K = 0$ for all $u \in H_0$. Thus, $\langle T^*(Tu_0 - \boldsymbol{f}), u\rangle_H = 0$ for all $u \in H_0$. Hence, $T^*Tu_0 - T^*\boldsymbol{f} = 0$. The expression for the solution $u_0 \in H_0$ in Equation (4.2) follows from (2.12) and (2.13). □

REMARK 4.2. Whereas the equation $T^*Tu = T^*\boldsymbol{f}$ written in expanded form as (4.1) is an equation between well-defined measurable functions, the equation $S^*S\,u = S^*\boldsymbol{f}$, which we can write in the apparently simpler expanded form as

$$(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla}u\rangle = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{f}\rangle,$$

is an equation between generalised functions. Despite this distinction, the two equations are mathematically equivalent. For numerical mathematicians it may be more useful to express the key equation in the form (4.1). This means the adequacy of an approximate solution $u_\epsilon \approx u_0$ could be checked by calculating the error $\epsilon = T^*Tu_\epsilon - T^*\boldsymbol{f} \approx 0$.

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5. A hypothetical example

In this section we will illustrate our general remarks by considering a special case. Since much of the familiar Sturm–Liouville theory arises in the context of a transformation to orthogonal curvilinear coordinates, we begin by reviewing the basic formulæ. Let $\boldsymbol{y} = (y_1, y_2, y_3) \in \mathbb{R}^3$ be the usual rectangular coordinates and let $\boldsymbol{z} = (z_1, z_2, z_3)$ be an alternative system of orthogonal curvilinear coordinates. If we consider the functional dependence $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{z})$, then the curvilinear coordinates are defined by the unit vectors

$$\boldsymbol{f}_i(\boldsymbol{z}) = (1/h_i)\partial_i \boldsymbol{y},$$

where $h_i = h_i(\boldsymbol{z}) = \|\partial_i \boldsymbol{y}(\boldsymbol{z})\| = \|\partial_i \boldsymbol{y}\|$ for each $i = 1, 2, 3$. We have $\langle \boldsymbol{f}_i, \boldsymbol{f}_j \rangle = \delta_{ij}$ and the gradient vector is given by

$$\boldsymbol{\nabla} u = \sum_{i=1}^{3} (1/h_i)\partial_i u \boldsymbol{f}_i,$$

while the divergence can be calculated from

$$\langle \boldsymbol{\nabla}, \boldsymbol{\psi} \rangle = 1/(h_1 h_2 h_3) \sum_{i=1}^{3} \partial_i (h_{j(i)} h_{k(i)} \psi_i),$$

where $j(i) < k(i)$ and $j(i), k(i) \neq i$. Thus,

$$(-1)\langle \boldsymbol{\nabla}, \boldsymbol{\nabla} u \rangle = (-1)(1/(h_1 h_2 h_3)) \sum_{i=1}^{3} \partial_i ((1/h_i) h_{j(i)} h_{k(i)} \partial_i u),$$

where $j(i) < k(i)$ and $j(i), k(i) \neq i$. We can reproduce these formulæ using the operator $L = (-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla} \rangle$ by choosing $p(\boldsymbol{x}) = h_1(\boldsymbol{x}) h_2(\boldsymbol{x}) h_3(\boldsymbol{x})$ and

$$W(\boldsymbol{x}) = \begin{pmatrix} h_2(\boldsymbol{x})h_3(\boldsymbol{x})/h_1(\boldsymbol{x}) & 0 & 0 \\ 0 & h_1(\boldsymbol{x})h_3(\boldsymbol{x})/h_2(\boldsymbol{x}) & 0 \\ 0 & 0 & h_1(\boldsymbol{x})h_2(\boldsymbol{x})/h_3(\boldsymbol{x}) \end{pmatrix}.$$

Example 5.1. Let $\Omega = \{\boldsymbol{x} \mid \boldsymbol{x} \in (-1, 1) \times (0, 1)^2\}$ and define the weight functions $p(\boldsymbol{x}) = \pi/(x_2 \sqrt{1 - x_1^2})$ and

$$W(\boldsymbol{x}) = \begin{pmatrix} \pi \sqrt{1 - x_1^2}/x_2 & 0 & 0 \\ 0 & \pi x_2 \Big/ \sqrt{1 - x_1^2} & 0 \\ 0 & 0 & 1 \Big/ \Big(\pi x_2 \sqrt{1 - x_1^2}\Big) \end{pmatrix}$$

for all $\boldsymbol{x} \in \Omega$. In order to solve the equation $(-1)(1/p)\langle \boldsymbol{\nabla}, W\boldsymbol{\nabla} u \rangle = \sigma^2 u$ by separation of variables, we set $u(\boldsymbol{x}) = u_1(x_1) u_2(x_2) u_3(x_3)$ and obtain

$$(-1)\Big[\frac{\sqrt{1 - x_1^2}}{u_1}\, \partial_1 \Big(\sqrt{1 - x_1^2} \cdot u_1'\Big) + \frac{x_2}{u_2}\, \partial_2 (x_2 u_2') + \frac{1}{\pi u_3}\, \partial_3 \Big(\frac{u_3'}{\pi}\Big)\Big] = \sigma^2.$$

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For the first variable, we have a Chebyshev equation

$$-(1-x_1^2)\frac{u''_{1,\ell}}{u_{1,\ell}} + x_1\frac{u'_{1,\ell}}{u_{1,\ell}} = (\ell+1)^2$$

with $u_{1,\ell}(-1) = 0$ and $u_{1,\ell}(1) = 0$ for each $\ell \in \mathbb{N}$. The solution is given by

$$u_{1,\ell}(x_1) = \sin(\ell \arccos x_1) = \sqrt{1-x_1^2} \cdot U_\ell(x_1),$$

where U_ℓ is the Chebyshev polynomial of the second kind of degree ℓ. For the second variable, the separation leads to a Bessel equation

$$-\frac{u''_{2,m}}{u_{2,m}} - \frac{1}{x_2}\frac{u'_{2,m}}{u_{2,m}} = \mu_m^2$$

with $u_{2,m}(0) = 0$ and $u_{2,m}(1) = 0$ for each $m \in \mathbb{N}$. The solution is given by

$$u_{2,m} = J_0(\mu_m x_2),$$

where J_0 is the Bessel function of the first kind of order 0 and where $\{\mu_m\}_{m\in\mathbb{N}}$ with $0 < \mu_m < \mu_{m+1}$ are all the solutions to the equation $J_0(x) = 0$ in the region $x > 0$. The equation for the third variable is a standard trigonometric equation

$$-\frac{1}{\pi^2}\frac{u''_{3,n}}{u_{3,n}} = n^2$$

with $u_{3,n}(0) = 0$ and $u_{3,n}(1) = 0$ for each $n \in \mathbb{N}$. The solution is given by

$$u_{3,n}(x_3) = \sin n\pi x_3.$$

Hence, the complete set of orthogonal eigenfunctions for S^*S is given by

$$u_{\ell,m,n}(\boldsymbol{x}) = \sqrt{1-x_1^2} \cdot U_\ell(x_1) J_0(\mu_m x_2) \sin n\pi x_3$$

with corresponding eigenvalues

$$\sigma_{\ell,m,n}^2 = (\ell+1)^2 + \mu_m^2 + n^2$$

for $(\ell, m, n) \in \mathbb{N}^3$. Thus, we seek a solution $u_0 \in H_0$ to the equation $T^*Tu = T^*\boldsymbol{f}$ in the form

$$u = \sum_{(\ell,m,n)\in\mathbb{N}^3} c_{\ell,m,n} u_{\ell,m,n},$$

where $c_{\ell,m,n} \in \mathbb{C}$. It follows from Equations (2.12) and (2.13), using the notation established earlier in the paper, that the solution is

$$u_0 = \sum_{(\ell,m,n)\in\mathbb{N}^3} \langle \boldsymbol{f}, \boldsymbol{w}_{\ell,m,n}\rangle_K \Big(\sqrt{\sigma_{\ell,m,n}^2 + 1}/\sigma_{\ell,m,n}\Big) u_{\ell,m,n} \in H_0.$$

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6. Conclusions

We have shown that the potential function that generates the best gradient approximation to an observed square integrable function on a bounded measurable set subject to a condition that the boundary potential is zero satisfies a classical self-adjoint linear elliptic differential equation. The method relies on formulation of the gradient operator as a bounded linear operator on an appropriate Sobolev space. We have also shown how our analysis is closely linked to the traditional solution of self-adjoint linear elliptic differential equations where an unbounded gradient operator is normally used. In practical applications the proposed gradient approximation procedure could be used to eliminate measurement errors when constructing a legitimate potential function to match an observed gradient. It should also enable numerical mathematicians to check an approximate numerical solution $u_\epsilon(\boldsymbol{x}) \approx u_0(\boldsymbol{x})$ by calculating the error function $\epsilon(\boldsymbol{x}) = T^*Tu_\epsilon(\boldsymbol{x}) - T^*f(\boldsymbol{x}) \approx 0$.

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