A Short Course on Duality, Adjoint Operators, Green's Functions, and A Posteriori *Error Analysis*

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Outline of this course

This course has four parts:

- Basic background and theory of the concepts of duality, adjoint operators, and Green's functions
- Development of an approach to *a posteriori* error analysis and adaptive error control based on a generalization of the Green's function
- An application of these ideas to using the effective domain of influence in elliptic problems to form a decomposition of a solution
- Extension of the ideas to nonlinear problems.

Duality, Adjoint Operators, and Green's Functions

The Green's Function

In the classic problem, u solves

$$\begin{cases} -\Delta u = f, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

where Ω is a domain in $\mathbb{R}^d$ with boundary $\partial\Omega$.

The Green's function ϕ satisfies

$$\begin{cases} -\Delta \phi(y;x) = \delta_y(x), & x \in \Omega, \\ \phi(y;x) = 0, & x \in \partial\Omega, \end{cases}$$

δ_y is the **delta function** at a point $y \in \Omega$.

The Green's Function

Function representation formula:

$$u(y) = \int_\Omega \delta_y(x) u(x)\, dx = \int_\Omega -\Delta\phi(y;x) u(x)\, dx$$

$$= \int_\Omega \phi(y;x) \cdot -\Delta u(x)\, dx = \int_\Omega \phi(y;x) f(x)\, dx.$$

Background in linear algebra

X is a vector space with norm $\| \, \|$ over the real numbers

An important property of the spaces depends on the notion of a Cauchy sequence:

Definition
A sequence $\{x_n\}$ in X is a **Cauchy sequence** if we can make the distance between elements in the sequence arbitrarily small by restricting the indices to be large.

More precisely, for every $\epsilon > 0$ there is an N such that $\|x_n - x_m\| < \epsilon$ for all $n, m > N$.

This is a computable criterion for checking convergence.

Background in linear algebra

Example
Consider the sequence $\{1/n\}_{n=1}^{\infty}$ in $[0,1]$. It is a Cauchy sequence since

$$\left|\frac{1}{n}-\frac{1}{m}\right| = \left|\frac{m-n}{mn}\right| \leq 2\frac{\max\{m,n\}}{mn} = \frac{2}{\min\{m,n\}}$$

can be made arbitrarily small by taking m and n large.

It converges to 0 which is in $[0,1]$.

Sequences that converge are Cauchy sequences. Cauchy sequences do not necessarily converge.

Example
The sequence $\{1/n\}_{n=1}^{\infty}$ is a Cauchy sequence in $(0,1)$ but does not converge in $(0,1)$.

Background in linear algebra

Spaces in which Cauchy sequences converge are greatly preferred.

Definition
A **Banach space** is a vector space with a norm such that every Cauchy sequence converges to a limit in the space.

We also say the space is **complete**.

Background in linear algebra

Example

$\mathbb{R}^n$ with the norms defined for $x = (x_1, \cdots, x_n)^\top$,

$$\|x\|_1 = |x_1| + \cdots + |x_n|$$

$$\|x\|_2 = \left(|x_1|^2 + \cdots + |x_n|^2\right)^{1/2}$$

$$\|x\|_\infty = \max |x_i|.$$

are all Banach spaces.

We use $\| \ \| = \| \ \|_2$ unless noted otherwise.

Background in linear algebra

Spaces of functions:

Definition
For an interval $[a, b]$, the space of continuous functions is denoted $C([a, b])$, where we take the maximum norm

$$\|f\| = \max_{a \le x \le b} |f(x)|.$$

$C^1([a, b])$ denotes the space of functions that have continuous first derivatives on $[a, b]$, where we use the norm

$$\|f\| = \max_{a \le x \le b} |f(x)| + \max_{a \le x \le b} |f'(x)|.$$

Background in linear algebra

Spaces of functions:

Definition
For $1 \leq p \leq \infty$,

$$L^p(\Omega) = \{f : f \text{ is measurable on } \Omega \text{ and } \|f\|_p < \infty\}$$

where for $1 \leq p < \infty$,

$$\|f\|_p = \left(\int_\Omega \|f\|^p \, dx\right)^{1/p}, \; 1 \leq p < \infty, \text{ and } \quad \|f\|_\infty = \text{ess sup}_\Omega \|f\|.$$

L^2 is particularly important.

Background in linear algebra

Theorem
The L^p spaces and $C([a,b])$ are Banach spaces.

Background in linear algebra

Consider two vector spaces X and Y with norms $\| \|_X$ and $\| \|_Y$

Definition
A **map** or **operator** L from X to Y is a rule or association that assigns to each x in X a unique element y in Y.

Definition
A map $L : X \to Y$ is **linear** if $L(\alpha x_1 + \beta x_2) = \alpha L(x_1) + \beta L(x_2)$ for all numbers α, β and x_1, x_2 in X.

Background in linear algebra

Example
Every linear map from $\mathbb{R}^m$ to $\mathbb{R}^n$ is obtained by multiplying vectors in $\mathbb{R}^m$ by a $n \times m$ matrix, i.e., they have the form Ax, where A is a $n \times m$ matrix.

Example
Differentiation is a linear map from $C^1([a,b])$ to $C([a,b])$.

Background in linear algebra

The maps we consider also have to behave continuously.

Definition
A map $L : X \to Y$ is **continuous** if for every sequence $\{x_n\}$ in X that converges to a limit x in X, i.e., $x_n \to x$, we have $L(x_n) \to L(x)$.

Example
Linear maps from $\mathbb{R}^m$ to $\mathbb{R}^n$ are continuous.

Background in linear algebra

There is an equivalent property for linear maps.

Definition
A linear map $L : X \to Y$ is **bounded** if there is a constant $C > 0$ such that $\|Lx\|_Y \leq C\|x\|_X$ for all x in X.

Theorem
A linear map between normed vector spaces is continuous if and only if it is bounded.

Background in linear algebra

The set of all linear transformations between two vector spaces X and Y is a vector space.

Definition
If X and Y are normed vector spaces, we use $\mathcal{L}(X, Y)$ to denote the vector space of all *bounded* linear maps from X to Y.
$\mathcal{L}(X, Y)$ is a normed vector space under the **operator norm**

$$\|L\| = \sup_{\|x\|_X = 1} \|Lx\|_Y = \sup_{x \neq 0} \frac{\|Lx\|_Y}{\|x\|_X}. \tag{1}$$

Background in linear algebra

Example

If the linear transformation L is given by the $n \times n$ matrix A, then

$$\|L\|_1 = \|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{n} |a_{ij}|$$

$$\|L\|_2 = \|A\|_2 = \sqrt{\sigma(A^T A)}$$

$$\|L\|_\infty = \|A\|_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$$

where $\sigma(A^\top A)$ is the spectral radius of $A^\top A$.

Background in linear algebra

Theorem
If X and Y are normed vector spaces and Y is complete, then $\mathcal{L}(X, Y)$ is complete.

Linear functionals and dual spaces

The concept of duality starts with linear functionals.

Definition
A **linear functional** on a vector space X is a linear map from X to $\mathbb{R}$.

Example
Let v in $\mathbb{R}^n$ be fixed. The map $F(x) = v \cdot x = (x, v)$ is a linear functional on $\mathbb{R}^n$.

Example
Consider $C([a, b])$. Both $I(f) = \int_a^b f(x)\,dx$ and $F(f) = f(y)$ for $a \leq y \leq b$ are linear functionals.

Linear functionals and dual spaces

A linear functional provides a "low dimensional snapshot" of a vector.

Example

In the example above with $F(x) = (x, v)$, consider $v = e_i$, the ith standard basis function. Then $F(x) = x_i$ where $x = (x_1, \cdots, x_n)$.

We can take $v = (1, 1, \cdots, 1)/n$ and compute the average of the components of a given input vector.

Linear functionals and dual spaces

Example

δ_y gives a linear functional on sufficiently smooth, real valued functions via

$$F(u) = u(y) = \int_\Omega \delta_y(x) u(x)\, dx.$$

Another linear functional is the average value of an integrable function,

$$F(u) = \frac{1}{\text{vol. of } \Omega} \int_\Omega u(x)\, dx.$$

We can view the formulas defining the Fourier coefficients of a function as a set of linear functionals.

Linear functionals and dual spaces

We are interested in the continuous linear functionals.

Definition
If X is a normed vector space, the space $\mathcal{L}(X, \mathbb{R})$ of bounded linear functionals on X is called the **dual space of** or **on** or **to** X, and is denoted by X^*.

The dual space is a normed vector space under the **dual norm** defined for $y \in X^*$ as

$$\|y\|_{X^*} = \sup_{\substack{x \in X \\ \|x\|_X = 1}} |y(x)| = \sup_{\substack{x \in X \\ x \neq 0}} \frac{|y(x)|}{\|x\|}.$$

Linear functionals and dual spaces

Example

Consider $X = \mathbb{R}^n$. Every vector v in $\mathbb{R}^n$ is associated with a linear functional $F_v(\cdot) = (\cdot, v)$. This functional is clear bounded since $|(x, v)| \leq \|v\| \, \|x\|$ (The "C" in the definition is $\|v\|$).

A classic result in linear algebra is that *all* linear functionals on $\mathbb{R}^n$ have this form, i.e., we can make the identification $(\mathbb{R}^n)^* \simeq \mathbb{R}^n$.

Linear functionals and dual spaces

Example

For $C([a,b])$, consider $I(f) = \int_a^b f(x)\,dx$. It is easy to compute

$$\|I\|_{C([a,b])^*} = \sup_{\substack{f \in C([a,b]) \\ \max|f|=1}} \left| \int_a^b f(x)\,dx \right|$$

by looking at a picture.

Linear functionals and dual spaces

Computing the dual norm of the integration functional.

The maximum value for $I(f)$ is clearly given by $f = 1$ or $f = -1$, and we get $\|I\|_{C([a,b])^*} = b - a$.

Linear functionals and dual spaces

Example

Recall Hölder's inequality for $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$ with $\frac{1}{p} + \frac{1}{q} = 1$ for $1 \leq p, q \leq \infty$ is

$$\|fg\|_{L^1(\Omega)} \leq \|f\|_{L^p(\Omega)} \|g\|_{L^q(\Omega)}.$$

Linear functionals and dual spaces

Each g in $L^q(\Omega)$ is associated with a bounded linear functional on $L^p(\Omega)$ when $\frac{1}{p} + \frac{1}{q} = 1$ and $1 \leq p, q \leq \infty$ by

$$F(f) = \int_\Omega g(x) f(x)\, dx.$$

We can "identify" $(L^p)^*$ with L^q when $1 < p, q < \infty$, The cases $p = 1, q = \infty$ and $p = \infty, q = 1$ are trickier.

The case L^2 is special in that we can identify $(L^2)^*$ with L^2.

Linear functionals and dual spaces

The dual space is the collection of "reasonable" possible samples.

An important characteristic of a dual space is how much we can reveal about a vector by considering samples in the dual space.

Example
By considering the set of n functionals corresponding to taking the inner product with $\{e_1, \cdots, e_n\}$, we can "reconstruct" any given vector in $\mathbb{R}^n$ by looking at the functional values.

The question of whether or not we can "recover" a vector u completely by computing sufficiently many linear functionals depends heavily on properties of the underlying space.
In practice, we will often be content with one or just a few "snapshots".

Linear functionals and dual spaces

We might wonder about the number of bounded linear functionals that exist on an arbitrary normed vector space.

The celebrated Hahn-Banach theorem says there is a great abundance of them.

Let $x_0 \neq 0$ be a fixed element of Banach space X.

The set $X_0 = \{\alpha x_0 : \alpha \in \mathbb{R}\}$ forms a vector subspace of X.

The linear functional $F(\alpha x_0) = \alpha$ is defined on X_0 and is bounded since $|F(\alpha x_0)| = |\alpha| = \|\alpha x_0\|/\|x\|$.

So, we have found a bounded linear functional on a subspace of X.

Can we extend this to be defined on all of X?

Linear functionals and dual spaces

Issues:

- What does it mean to extend?
- Does the norm increase upon extension?
- What if there is an infinite number of extensions involved?

Theorem
Hahn-Banach Let X be a Banach space and X_0 a subspace of X. Suppose that $F_0(x)$ is a bounded linear functional defined on X_0. There is a linear functional F defined on X such that $F(x) = F_0(x)$ for x in X_0 and $\|F\| = \|F_0\|$.

Linear functionals and dual spaces

Dual spaces are connected to distribution theory and weak convergence.

The dual space can be better behaved than the original normed vector space.

Theorem
If X is a normed vector space over $\mathbb{R}$, then X^* is a Banach space (whether or not X is a Banach space).

Linear functionals and dual spaces

Useful notation:

Definition
If x is in X and y is in X^*, we denote the value

$$y(x) =< x, y > .$$

This is called the **bracket notation**.

Linear functionals and dual spaces

The norms on X and its dual X^* are closely related. Recall that if $y \in X^*$, then

$$\|y\|_{X^*} = \sup_{\substack{x \in X \\ \|x\|_X = 1}} |y(x)| = \sup_{\substack{x \in X \\ x \neq 0}} \frac{|y(x)|}{\|x\|}.$$

Linear functionals and dual spaces

Definition
The **generalized Cauchy inequality** is

$$|< x, y >| \leq \|x\|_X \, \|y\|_{X^*}, \quad x \in X, \, y \in X^*.$$

Theorem
If X is a Banach space, then

$$\|x\|_X = \sup_{\substack{y \in X^* \\ y \neq 0}} \frac{|y(x)|}{\|y\|_{X^*}} = \sup_{\substack{y \in X^* \\ \|y\|_{X^*} = 1}} |y(x)|$$

for all x in X.

Hilbert spaces and duality

Example
$\mathbb{R}^n$ with the standard Euclidean norm $\| \, \| = \| \, \|_2$ can be identified with its dual space.

L^2 can be identified with its dual space.

Both of these spaces are Hilbert spaces.

Hilbert spaces and duality

One way to get a normed vector space is to place an inner product (i.e., dot product) on the space.

Theorem
If X has an inner product (x, y), then it is a normed vector space with norm $\|x\| = (x, x)^{1/2}$ for x in X.

Definition
A vector space with an inner product that is a Banach space with respect to the associated norm is called a **Hilbert** space.

Example
$\mathbb{R}^n$ with $\| \, \| = \| \, \|_2$ and L^2 are both Hilbert spaces.

Hilbert spaces and duality

If X is a Hilbert space with inner product (x, y), then each $y \in X$ determines a linear functional $F_y(x) =< x, y >= (x, y)$ for x in X.

This functional is bounded by Cauchy's inequality, $|(x, y)| \leq \|x\| \, \|y\|$.

The Riesz Representation theorem says this is the only kind of linear functional on a Hilbert space.

Theorem
Riesz Representation For every bounded linear functional F on a Hilbert space X, there is a *unique* element y in X such that

$$F(x) = (x, y), \text{ all } x \in X \text{ and } \|y\|_{X^*} = \sup_{\substack{x \in X \\ x \neq 0}} \frac{|F(x)|}{\|x\|}.$$

Hilbert spaces and duality

A Hilbert space is isometric to its dual space.

Definition
Two normed vector spaces X and Y are **isometric** if there is a linear 1-1 and onto map $L : X \to Y$ such that $\|L(x)\|_Y = \|x\|_X$ for all x in X.

We often replace the bracket notation and the generalized Cauchy inequality by the inner product and the “real” Cauchy inequality without comment.

Hilbert spaces and duality

The Sobolev spaces are Hilbert spaces based on L^2.

Example

For $k = 1, 2, 3, \cdots$, we define $H^k(\Omega)$ to be the *distribution* functions in $L^2(\Omega)$ whose partial derivatives of order k and less are also distributions in $L^2(\Omega)$.

Hilbert spaces and duality

Definition
index notation: For $\alpha = (\alpha_1, \cdots, \alpha_n)$ with integer coefficients, we define

$$D = \left(\frac{\partial}{\partial x_1}, \cdots, \frac{\partial}{\partial x_n} \right), \qquad D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}$$

with $|\alpha| = \alpha_1 + \cdots + \alpha_n$.

$H^k(\Omega) = \{u, D^\alpha u \in L^2(\Omega), |\alpha| \leq k\}$. The inner products and norms are

$$(u, v)_k = \sum_{|\alpha| \leq k} (D^\alpha u, D^\alpha v), \quad \|u\|_k = (u, u)_k^{1/2}.$$

Hilbert spaces and duality

The Riesz Representation theorem says that every linear functional on H^k has the form $(u, v)_k$ for some fixed v in H^k.

Defining the dual space to H^k runs into subtle difficulties due to a collision with the requirements for using distribution theory.

We define the dual spaces to a subspace.

$$H_0^k(\Omega) = \left\{ u \in H^k(\Omega) : u = \frac{\partial u}{\partial n} = \cdots = \frac{\partial^{k-1} u}{\partial n^{k-1}} = 0 \text{ on } \partial\Omega \right\},$$

where $\partial/\partial n$ denotes the normal derivative on the boundary $\partial\Omega$.

We let $H^{-k}(\Omega)$ is the set of all linear functionals on $H_0^k(\Omega)$.

Adjoint operators - definition

We now explain how a linear transformation between two normed vector spaces X and Y is naturally associated with another linear transformation between Y^* and X^*.

This is the infamous adjoint operator.

Adjoint operators - definition

Suppose $L \in \mathcal{L}(X, Y)$ is a bounded linear transformation.

For each $y^* \in Y^*$,

$$y^* \circ L(x) = y^*(L(x)) =< Lx, y^* >$$

assigns a number to each $x \in X$, hence defines a functional $F(x)$. $F(x)$ is clearly linear.

It is also bounded since

$$|F(x)| = |y^*(L(x))| \leq \|y^*\|_{Y^*} \|L(x)\|_Y \leq \|y^*\|_{Y^*} \|L\| \, \|x\|_X .$$

Adjoint operators - definition

There is an $x^* \in X^*$ such that $y^*(L(x)) = x^*(x)$ for all $x \in X$.

x^* is unique.

Thus, to each $y^* \in Y^*$, we have assigned a unique $x^* \in X^*$ and thus have defined a linear transformation $L^* : Y^* \to X^*$.

We can write these relations as

$$y^*(L(x)) = L^* y^*(x)$$

Adjoint operators - definition

Using the bracket notation,

$$< L(x), y^* >=< x, L^*(y^*) > \quad x \in X,\, y^* \in Y^*.$$

Definition
This is called the **bilinear identity**.

It defines the adjoint operator $L^* : Y^* \to X^*$ associated to a bounded linear transformation $L : X \to Y$.

Note that we have defined the adjoint transformation via sampling by elements in the dual space.

Adjoint operators - definition

Example
Let $X = \mathbb{R}^m$ and $Y = \mathbb{R}^n$, where we take the standard inner product and norm.

By the Riesz Representation theorem, the bilinear identity for $L \in \mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)$ reads

$$(Lx, y) = (x, L^* y), \quad x \in \mathbb{R}^m,\ y \in \mathbb{R}^n.$$

Adjoint operators - definition

There is a unique $n \times m$ matrix A so that if $y = L(x) = Ax$ where

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nm} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

and

$$y_i = \sum_{j=1}^{m} a_{ij} x_j, \quad 1 \leq i \leq n.$$

Adjoint operators - definition

For a linear functional $y^* = (y_1^*, \cdots, y_n^*)^\top \in Y^*$

$$L^* y^*(x) = y^*(L(x)) = \left((y_1^*, \cdots, y_n^*), \begin{pmatrix} \sum_{j=1}^m a_{1j} x_j \\ \vdots \\ \sum_{j=1}^m a_{nj} x_j \end{pmatrix} \right)$$

$$= \sum_{j=1}^m y_1^* a_{1j} x_j + \cdots \sum_{j=1}^m y_n^* a_{nj} x_j$$

$$= \sum_{j=1}^m \left(\sum_{i=1}^n y_i^* a_{ij} \right) x_j$$

Adjoint operators - definition

$L^*(y^*)$ is given by the inner product with $\tilde{y} = (\tilde{y}_1, \cdots, \tilde{y}_m)^\top$ where

$$\tilde{y}_j = \sum_{i=1}^{n} y_i^* a_{ij}.$$

Adjoint operators - definition

The matrix A^* of L^* is

$$A^* = \begin{pmatrix} a_{11}^* & \cdots & a_{1n}^* \\ \vdots & & \vdots \\ a_{m1}^* & \cdots & a_{mn}^* \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ \vdots & & & \vdots \\ a_{1m} & a_{2m} & \cdots & a_{nm} \end{pmatrix} = A^\top.$$

The bilinear identity is

$$y^\top A x = x^\top A^\top y$$

using the fact that $(x, y) = (y, x)$.

Adjoint operators - definition

The following theorem is crucial.

Theorem

$L^* \in \mathcal{L}(Y^*, X^*)$ and $\|L^*\| = \|L\|$.

proof

$$|L^* y^*(x)| \leq \|y^*\|_{Y^*} \|L\| \|x\|_X .$$

Therefore,

$$\|L^* y^*\|_{X^*} = \sup_{x \neq 0} \frac{|L^* y^*(x)|}{\|x\|} \leq \|y^*\|_{Y^*} \|L\|,$$

which implies that $L^* \in \mathcal{L}(Y^*, X^*)$ and $\|L^*\| \leq \|L\|$.

Adjoint operators - definition

To show the reverse inequality, we prove that

$$\|Lx\|_Y \leq \|L^*\| \, \|x\|_X, \quad x \in X.$$

The bilinear identity implies that

$$|y^*(Lx)| \leq \|L^* y^*\|_{X^*} \|x\|_X \leq \|L^*\| \|y^*\|_{Y^*} \|x\|_X$$

and

$$\sup_{y^* \neq 0} \frac{|y^*(Lx)|}{\|y^*\|_{Y^*}} \leq \|L^*\| \, \|x\|_X, \quad x \in X.$$

Adjoint operators - definition

Properties of the adjoint operator:

Theorem
Let X, Y, and Z be normed linear spaces. Then,

$$0^* = 0$$

$$(L_1 + L_2)^* = L_1^* + L_2^*, \quad \text{all } L_1, L_2 \in \mathcal{L}(X, Y)$$

$$(\alpha L)^* = \alpha L^*, \quad \text{all } \alpha \in \mathbb{R},\ L \in \mathcal{L}(X, Y)$$

If $L_2 \in \mathcal{L}(X, Y)$ and $L_1 \in \mathcal{L}(Y, Z)$, then $L_1 L_2 \in \mathcal{L}(X, Z)$, $(L_1 L_2)^* \in \mathcal{L}(Z^*, X^*)$, and

$$(L_1 L_2)^* = L_2^* L_1^*.$$

Adjoint operators - definition

We are often deal with linear operators that are not defined on the entire space.

Example
Consider $D = d/dx$ on $X = C([0,1])$. This linear map is only defined on the subspace $C^1([0,1])$.

Adjoint operators - definition

Definition
Let X and Y be normed vector spaces. A map L that assigns to each x in a subset $\mathcal{D}(L)$ of X a unique element y in Y is called a **map** or **operator** with **domain** $\mathcal{D}(L)$.

L is **linear** if (1) $\mathcal{D}(L)$ is a vector subspace of X and (2) $L(\alpha x_1 + \beta x_2) = \alpha L(x_1) + \beta L(x_2)$ for all $\alpha, \beta \in \mathbb{R}$ and $x_1, x_2 \in \mathcal{D}(L)$.

Adjoint operators - definition

We define the dual of a linear operator by examining its behavior on its domain.

We want

$$L^* y^*(x) = y^*(Lx) \quad \text{all } x \in \mathcal{D}(L).$$

We say that $y^* \in \mathcal{D}(L^*)$ if there is an $x^* \in X^*$ such that

$$x^*(x) = y^*(Lx), \quad \text{all } x \in \mathcal{D}(L).$$

The existence of x^* is no longer automatic.

When x^* exists, we define $L^* y^* = x^*$.

Adjoint operators - definition

For this to work, x^* must be unique.

In other words, $x^*(x) = 0$ for all $x \in \mathcal{D}(L)$ should imply $x^* = 0$.

This depends on the "size" of $\mathcal{D}(L)$.

Definition
A subspace A of a normed linear space X is **dense** if every point in X is either in A or the limit of a sequence of points in A.

Example
The rational numbers are dense in the real numbers and the polynomials are dense in $C([a, b])$.

Adjoint operators - definition

We can define L^* for a linear operator $L : X \to Y$ provided $\mathcal{D}(L)$ is dense in X.

We define $\mathcal{D}(L^*)$ to be those $y^* \in Y^*$ for which there is an $x^* \in X^*$ with $x^*(x) = y^*(Lx)$ for all $x \in X$.

This x^* is unique and $L^* y^* = x^*$.

The Hahn-Banach theorem implies that if there is a C such that $|y^*(Lx)| \leq C\|x\|$ for all $x \in \mathcal{D}(L)$, then $y^* \in \mathcal{D}(L^*)$.

Adjoint operators - motivation

Common problem: Given normed vector spaces X and Y, an operator $\mathcal{L}(X, Y)$, and $b \in Y$, find $x \in X$ such that

$$Lx = b.$$

We explain the role of the adjoint in solving this kind of problems.

Adjoint operators - motivation

Definition
The set of b for which there is a solution is called the **range**, $\mathcal{R}(L)$, of L.

The set of x for which $L(x) = 0$ is called the **null space**, $\mathcal{N}(L)$, of L.

0 is always in $\mathcal{N}(L)$.

If it is the only element in $\mathcal{N}(L)$, then $Lx = b$ can have at most one solution.

Adjoint operators - motivation

Theorem
$\mathcal{N}(L)$ is a subspace of X and $\mathcal{R}(L)$ is a subspace of Y.

Adjoint operators - motivation

If $y \in \mathcal{R}(L)$, there is an x with $Lx = y$.

For $y^* \in Y^*$,

$$y^*(Lx) = y^*(y).$$

By the definition of the adjoint,

$$L^* y^*(x) = y^*(y).$$

If $y^* \in \mathcal{N}(L^*)$, then $y^*(y) = 0$.

A necessary condition that $y \in \mathcal{R}(L)$ is that $y^*(y) = 0$ for all $y^* \in \mathcal{N}(L^*)$.

Adjoint operators - motivation

Is this sufficient?

We require just one condition.

Definition
A subset A of a normed vector space X is **closed** if every sequence $\{x_n\}$ in A that has a limit in X has its limit in A.

Theorem
Let X and Y be normed linear spaces and $L \in \mathcal{L}(X, Y)$. A necessary condition that $y \in \mathcal{R}(L)$ is $y^*(y) = 0$ for all $y^* \in \mathcal{N}(L^*)$. This is a sufficient condition if $\mathcal{R}$ is closed in Y.

Adjoint operators - motivation

Example
Suppose that $L \in \mathcal{L}(X, Y)$ is associated with the $n \times m$ matrix A, i.e., $L(x) = Ax$.

The necessary and sufficient condition for the solvability of $Ax = b$ is that b is orthogonal to all linearly independent solutions of $A^T y = 0$.

Adjoint operators - motivation

Example
In the case X is a Hilbert space and $L \in \mathcal{L}(X, Y)$, then necessarily $\mathcal{R}(L^*) \subset \mathcal{N}(L)^\perp$, where $S^\perp$ is the subspace of vectors that are orthogonal to a subspace S.

If $\mathcal{R}(L^*)$ is "large", then $\mathcal{N}(L)^\perp$ must be "large" and $\mathcal{N}(L)$ must be "small".

The existence of sufficiently many solutions of the homogeneous adjoint equation implies there is at most one solution of $Lx = b$ for a given b.

Adjoint operators - motivation

Example
The setting of general partial differential equations:

Theorem
Holmgren Uniqueness The generalized initial value problem consisting of the equation

$$L(u) = \sum_{|\alpha| \leq m} A_\alpha(x) D^\alpha u = f(x), \quad x \in \mathbb{R}^n,$$

where $\{A_\alpha\}$ and f are analytic functions, together with the data

$$D^\beta u(x) = g_\beta(x), \quad |\beta| \leq m-1, \, x \in S$$

given on an analytic noncharacteristic surface S, has at most one solution in a neighborhood of S.

Adjoint operators - motivation

The adjoint has an important role in the solution of a general $n \times m$ system $Ax = b$, where A is a $n \times m$ matrix, $x \in \mathbb{R}^m$, and $b \in \mathbb{R}^n$.

The reason to dwell on such problems is that differential operators do not tend to be “square”.

Example
$y'' = d^2y/dx^2$ requires two boundary conditions to define a problem for the associated differential equation that has a unique solution.

We may want to study the differential operator without any boundary conditions, or more or less than two conditions.

Adjoint operators - motivation

Example

Divergence,

$$\text{div}\, u = \frac{\partial u_1}{\partial x_1} + \cdots + \frac{\partial u_n}{\partial x_n},$$

associates a scalar with a given vector function, and the associated differential equation is very “under-determined”.

The gradient,

$$\text{grad}\, u = \left(\frac{\partial u_1}{\partial x_1}, \cdots, \frac{\partial u_n}{\partial x_n} \right),$$

associates a vector field with a given scalar function, and the associated equations are very “over-determined”.

Adjoint operators - motivation

Consider the $n \times m$ system $Ax = b$, where A is a $n \times m$ matrix, $x \in \mathbb{R}^m$, and $b \in \mathbb{R}^n$.

We enlarge the system by adding the adjoint $m \times n$ system $A^\top y = c$, where y and c are independent of x and b.

The new problem is an $(n+m) \times (n+m)$ symmetric problem

$$Sz = d,$$

with

$$z = \begin{pmatrix} y \\ x \end{pmatrix}, \quad d = \begin{pmatrix} b \\ c \end{pmatrix}, \quad S = \begin{pmatrix} 0 & A \\ A^\top & 0 \end{pmatrix}.$$

Adjoint operators - motivation

Since S is symmetric, it is diagonalizable with eigenvalues satisfying

$$\begin{aligned} Av &= \lambda u \\ A^* u &= \lambda v \end{aligned} \qquad \text{or} \qquad \begin{aligned} AA^\top u &= \lambda^2 u \\ A^\top A v &= \lambda^2 v \end{aligned}$$

The eigenvalues of S are the singular values of A and last two equations give the left and right singular vectors of A.

Adjoint operators - motivation

Consequences:

- The theorem on the adjoint condition for solvability falls out right away.
- It yields a “natural” definition of a solution or gives conditions for a solution to exist in the over-determined and under-determined cases.
- It also gives a way of determining the condition of the solution process.

Adjoint operators - motivation

One interesting observation is that there is a reciprocal relationship between the degree of over/under-determination of the original system and the adjoint system.

The more over-determined the original system, the more under-determined the adjoint system, and so forth.

Adjoint operators - motivation

Example

Consider $2x_1 + x_2 = 4$, where $L : \mathbb{R}^2 \to \mathbb{R}$. $L^* : \mathbb{R} \to \mathbb{R}^2$ is given by $L^* = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$. The extended system is

$$\begin{pmatrix} 0 & 2 & 1 \\ 2 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ c_1 \\ c_2 \end{pmatrix},$$

from which we see that $2c_1 = c_2$ is required in order to have a solution.

Adjoint operators - motivation

Example

On the other hand, if the problem is

$$\begin{aligned} 2x_1 + x_2 &= 4 \\ x_2 &= 3, \end{aligned}$$

with $L : \mathbb{R}^2 \to \mathbb{R}^2$, then there is a unique solution. The extended system is

$$\begin{pmatrix} 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 1 \\ 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ 4 \\ 3 \end{pmatrix},$$

where we can specify any values for c_1, c_2.

Adjoint operators - motivation

In the under-determined case, we can eliminate the deficiency by posing the method of solution

$$\begin{aligned} AA^\top y &= b \\ x &= A^\top y. \end{aligned} \qquad \text{or} \qquad \begin{aligned} L(L^*(y)) &= b \\ x &= L^*(y). \end{aligned}$$

Adjoint operators - motivation

This works for differential operators

Example
Consider the under-determined problem

$$\text{div}\, F = \rho.$$

The adjoint to div is -grad modulo boundary conditions.

If $F = \text{grad}\, u$, where u is subject to the boundary condition $u(''\infty'') = 0$, then we obtain the "square", well-determined problem

$$\text{div grad}\, u = \Delta u = -\rho,$$

which has a unique solution because of the boundary condition.

Adjoint operators - motivation

Example
Consider

$$Ax = b$$

$$A^\top \phi = e_i$$

where A is a $n \times n$ invertible matrix.

There are no constraints on the data for the adjoint problem.

We have specified the ith standard basis vector of $\mathbb{R}^n$.

$$x_i = (x, e_i) = (x, A^\top \phi) = (Ax, \phi) = (b, \phi).$$

y is the discrete Green's vector associated to $Ax = b$.

Adjoint operators - computation

The computation of the adjoint to a general differential operator is not easy.

A tedious, formal approach:

1. Take the problem for the linear operator, including any boundary and/or initial conditions imposed with the operator, and discretize it.
2. Extract the matrix from the resulting discrete system, and compute its transpose.
3. Let the discretization parameter tend to its limit and determine the differential operator that is approached by the transposed matrix.

Determination of the adjoint of a differential operator is heavily influenced by the boundary and/or initial conditions, as well as the underlying spaces.

Adjoint operators - computation

Example
A standard difference approximation of

$$\begin{cases} -u''(x) = f(x), & 0 < x < 1, \\ u(0) = 0, u(1) = 0, \end{cases}$$

yields the matrix

$$\frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & -1 & 2 \end{pmatrix},$$

The differential operator is self-adjoint.

Adjoint operators - computation

Example

If we change the boundary conditions to

$$\begin{cases} -u''(x) = f(x), & 0 < x < 1, \\ u(0) = 0, u'(0) = 0, \end{cases}$$

we get a triangular matrix after discretization.

The adjoint corresponds to a problem

$$\begin{cases} -v''(x) = g(x), & 0 < x < 1, \\ v(1) = 0, v'(1) = 0, \end{cases}$$

Adjoint operators - computation

Example

$$\begin{cases} u' = f(x), & 0 < x < 1, \\ u(0) = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} -v' = g(x), & 1 > x > 0, \\ v(1) = 0, \end{cases}$$

Example

$$\begin{cases} -u'' = f(x), & 0 < x < 1, \\ \text{no boundary conditions} \end{cases}$$

$$\Rightarrow \quad \begin{cases} -v'' = g(x), & 0 < x < 1, \\ v(0) = v'(0) = v(1) = v'(1) = 0. \end{cases}$$

Adjoint operators - computation

In the case of L^2, we can use the bilinear identity

$$< Lu, v^* >=< u, L^* v^* > \quad \text{all } u \in X,\ v^* \in Y^*,$$

which is

$$(Lu, v) = (u, L^* v) \quad \text{all suitable } u, v \in L^2(\Omega).$$

Definition
We say that we are **evaluating the bilinear identity** when we compute

$$< Lu, v^* > - < u, L^* v^* >= (Lu, v) - (u, L^* v)$$

for some suitable functions u and v.

Adjoint operators - computation

- Since we are considering differential operators, these will not be defined on all of $L^2(\Omega)$, but only a subset of sufficiently smooth functions.
- The L^2 inner product involves integration over the domain, and we can interpret the process producing the bilinear identity as a succession of integration by parts. This yields terms that involve the integrals over the boundary of Ω of the functions involved as well as certain derivatives.

Adjoint operators - computation

Computing the adjoint using the bilinear identity proceeds in two stages.

First, we compute a formal adjoint neglecting all boundary terms by assuming that the functions involved have compact support inside Ω.

Definition
A function on a domain Ω has **compact support** in Ω if it vanishes identically outside a bounded set contained inside Ω.

Adjoint operators - computation

1. Take the differential operator applied to a smooth function with compact support and multiply by a smooth test function with compact support
2. Integrate over the domain
3. Integrate by parts to move all derivatives onto the test function while ignoring boundary terms.

Functions that have compact support are identically zero anywhere near the boundary and any boundary terms arising from integration by parts will vanish.

Adjoint operators - computation

Definition

Let L be a differential operator. The **formal adjoint** L^* is the differential operator that satisfies

$$(Lu, v) = (u, L^* v) \qquad \left(\int_\Omega Lu \cdot v \, dx = \int_\Omega u \cdot L^* v \, dx \right)$$

for all sufficiently smooth u and v with compact support in Ω.

Adjoint operators - computation

Example
Consider

$$Lu(x) = -\frac{d}{dx}\left(a(x)\frac{d}{dx}u(x)\right) + \frac{d}{dx}(b(x)u(x))$$

on $[0,1]$. Integration by parts neglecting boundary terms gives

$$\begin{aligned}
-\int_0^1 \frac{d}{dx}\left(a(x)\frac{d}{dx}u(x)\right) v(x)\,dx \\
&= \int_0^1 a(x)\frac{d}{dx}u(x)\frac{d}{dx}v(x)\,dx - a(x)\frac{d}{dx}u(x)v(x)\Big|_0^1 \\
&= -\int_0^1 u(x)\frac{d}{dx}\left(a(x)\frac{d}{dx}v(x)\right)\,dx + u(x)a(x)\frac{d}{dx}v(x)\Big|_0^1,
\end{aligned}$$

Adjoint operators - computation

$$\int_0^1 \frac{d}{dx}(b(x)u(x))v(x)\,dx = -\int_0^1 u(x)b(x)\frac{d}{dx}v(x)\,dx + b(x)u(x)v(x)\Big|_0^1,$$

where all of the boundary terms vanish.

Therefore,

$$L^*v = -\frac{d}{dx}\left(a(x)\frac{d}{dx}v(x)\right) - b(x)\frac{d}{dx}(v(x)).$$

Adjoint operators - computation

In higher space dimensions, we use the divergence theorem.

Example
A general linear second order differential operator L in $\mathbb{R}^n$ can be written

$$L(u) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x_i} + cu,$$

where $\{a_{ij}\}$, $\{b_i\}$, and c are functions of $x_1, x_2, \cdots, x_n$. Then,

$$L^*(u) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 (a_{ij} v)}{\partial x_i \partial x_j} - \sum_{i=1}^{n} \frac{\partial (b_i v)}{\partial x_i} + cv.$$

Adjoint operators - computation

It can be verified directly that

$$vL(u) - uL^*(v) = \sum_{i=1}^{n} \frac{\partial p_i}{\partial x_i},$$

where

$$p_i = \sum_{j=1}^{n} \left(a_{ij} v \frac{\partial u}{\partial x_j} - u \frac{\partial (a_{ij} v)}{\partial x_j} \right) + b_i u v.$$

The divergence theorem yields

$$\int_\Omega (vL(u) - uL^*(v))\, dx = \int_{\partial\Omega} p \cdot n \, ds = 0,$$

where $p = (p_1, \cdots, p_n)$ and n is the outward normal in $\partial\Omega$.

Adjoint operators - computation

A typical term,

$$va_{11}\frac{\partial^2 u}{\partial x_1^2} = va_{11}\frac{\partial}{\partial x_1}\left(\frac{\partial u}{\partial x_1}\right) = \frac{\partial}{\partial x_1}\left(va_{11}\frac{\partial u}{\partial x_1}\right) - \frac{\partial(a_{11}v)}{\partial x_1}\frac{\partial u}{\partial x_1}$$
$$= \frac{\partial}{\partial x_1}\left(va_{11}\frac{\partial u}{\partial x_1}\right) - \frac{\partial}{\partial x_1}\left(u\frac{\partial(a_{11}v)}{\partial x_1}\right) + u\frac{\partial^2(a_{11}v)}{\partial x_1^2}$$

yielding

$$va_{11}\frac{\partial^2 u}{\partial x_1^2} - u\frac{\partial^2(a_{11}v)}{\partial x_1^2} = \frac{\partial}{\partial x_1}\left(a_{11}v\frac{\partial u}{\partial x_1} - u\frac{\partial(a_{11}v)}{\partial x_1}\right).$$

Adjoint operators - computation

Example

Let L be a differential operator of order $2p$ of the form

$$Lu = \sum_{|\alpha|,|\beta|\leq p} (-1)^{|\alpha|} D^\alpha \big(a_{\alpha\beta}(x) D^\beta u\big),$$

then

$$L^* v = \sum_{|\alpha|,|\beta|\leq p} (-1)^{|\alpha|} D^\alpha \big(a_{\beta\alpha}(x) D^\beta v\big),$$

and L is elliptic if and only if L^* is elliptic.

Adjoint operators - computation

Some special cases.

$$\text{grad}^* = -\text{div}$$

$$\text{div}^* = -\text{grad}$$

$$\text{curl}^* = \text{curl}$$

$$Lu = \sum_{|\alpha| \leq p} a_\alpha(x) D^\alpha u$$

then

$$L^* v = \sum_{|\alpha| \leq p} (-1)^{|\alpha|} D^\alpha (a_\alpha(x) v(x)).$$

Adjoint operators - computation

Example

If

$$Lu = \rho u_{tt} - \nabla \cdot (a \nabla u) + bu$$

then $L^* = L$.

If

$$Lu = u_t - \nabla \cdot (a \nabla u) + bu$$

then

$$L^* v = -v_t - \nabla \cdot (a \nabla v) + bv$$

where time runs "backwards".

Adjoint operators - computation

This procedure also works for systems

Example
Let

$$L(\vec{u}) = A\vec{u}_x + B\vec{u}_y + C\vec{u},$$

where A, B, and C are $n \times n$ matrices, then

$$L^*(\vec{v}) = (-A^\top \vec{v})_x - (B^\top \vec{v})_y + C^\top v,$$

so that

$$\vec{v}^\top L\vec{u} - \vec{u}^\top L^* \vec{v} = \nabla \cdot (\vec{v}^\top A\vec{u}, \vec{v}^\top B\vec{u}).$$

Adjoint operators - computation

In the second stage of computing the adjoint, we deal with boundary conditions by removing the assumption that the functions involved have compact support.

Integration by parts yields additional terms involving integrals over the boundary of the functions involved and their derivatives.

We want to determine boundary conditions such that the bilinear identity still holds, e.g., such that any boundary terms that arise vanish.

Adjoint operators - computation

It turns out that the form of the boundary conditions imposed in the problem for L are important, but the values given for these conditions are not.

If the boundary conditions are not homogeneous, we make them so for the purpose of determining the adjoint.

Definition
The **adjoint boundary conditions** posed on the formal adjoint operator are the minimal conditions required to make the boundary terms that appear when evaluating the bilinear identity for general smooth functions vanish.

Adjoint operators - computation

Some of the boundary terms that appear when evaluating the bilinear identity will vanish because of the boundary conditions imposed in the original problem.

The point of this assumption is to make the formal adjoint serve as the true adjoint by pairing it with the correct boundary conditions.

Adjoint operators - computation

This definition can be made completely precise. Issues involved:

- Placing conditions on the differential operator L so that evaluating the bilinear identity for general smooth functions results in expressions involving only values on the boundary.
- Making precise the meaning of “minimal conditions” needed for the adjoint problem, and proving these always exist.

Adjoint operators - computation

Example

Consider Newton's equation of motion $s''(x) = f(x)$ with $x =$ "time", normalized with mass 1. First, suppose we assume $s(0) = s'(0) = 0$, and $0 < x < 1$. We have

$$s''v - sv'' = \frac{d}{dx}(vs' - sv')$$

and

$$\int_0^1 (s''v - sv'')\,dx = (vs' - sv')\Big|_0^1.$$

Adjoint operators - computation

The boundary conditions imply the contributions at $x = 0$ vanish, while at $x = 1$ we have

$$v(1)s'(1) - v'(1)s(1).$$

To insure this vanishes, we must have $v(1) = v'(1) = 0$. These are the adjoint boundary conditions.

Adjoint operators - computation

Example
Suppose instead we impose conditions such that at the mass returns to the origin with zero speed at $x = 1$.

This gives four boundary conditions
$s(0) = s'(0) = s(1) = s'(1) = 0$ on the original problem.

In this situation, all of the boundary terms are zero and no boundary conditions will be imposed on the adjoint.

Adjoint operators - computation

Solving the over-determined problem.

Example
Based on the discussion above, we require the data f to be orthogonal to the solution of the adjoint problem $v'' = 0$, which is $v = a + bx$.

Hence, f must be orthogonal in $L^2(0,1)$ to 1 and x.

Assume for example that $f(x) = a + bx + cx^2$. It is easy to see that $(f,1) = 0$ and $(f,x) = 0$ forces $a = c/6$ and $b = -c$.

Choosing $c = 1$ for example, means that $f(x) = 1/6 - x + x^2$.

Adjoint operators - computation

We solve the forward problem by integrating twice and using the boundary conditions at $x = 0$ to get a formula for the solution.

The resulting solution satisfies the conditions at $x = 1$ as well.

Adjoint operators - computation

Example
Since

$$\int_\Omega (u\Delta v - v\Delta u)\,dx = \int_{\partial\Omega} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right)\,ds,$$

the Dirichlet and Neumann boundary value problems for the Laplacian are their own adjoints.

Adjoint operators - computation

Example

Let $\Omega \subset \mathbb{R}^2$ be bounded with a smooth boundary and let $s =$ arclength along the boundary. Consider

$$\begin{cases} -\Delta u = f, & x \in \Omega, \\ \frac{\partial u}{\partial n} + \frac{\partial u}{\partial s} = 0, & x \in \partial\Omega. \end{cases}$$

Since

$$\int_\Omega (u\Delta v - v\Delta u)\, dx = \int_{\partial\Omega} \left(u \left(\frac{\partial v}{\partial n} - \frac{\partial v}{\partial s} \right) - v \left(\frac{\partial u}{\partial n} + \frac{\partial u}{\partial s} \right) \right) ds,$$

the adjoint problem is

$$\begin{cases} -\Delta v = g, & x \in \Omega, \\ \frac{\partial v}{\partial n} - \frac{\partial v}{\partial s} = 0, & x \in \partial\Omega. \end{cases}$$

Green's functions

For simplicity, we consider

$$\begin{cases} Lu = f, & x \in \Omega, \\ \text{suitable b.c. and i.v.}, & x \in \partial\Omega, \end{cases}$$

where L is a linear differential operator.

We specify the correct boundary and/or initial conditions so there is a unique solution.

Green's functions

Definition
The **Green's function** satisfies

$$\begin{cases} L^*\phi(y,x) = \delta_y(x), & x \in \Omega, \\ \text{adjoint b.c. and i.v.}, & x \in \partial\Omega, \end{cases}$$

where L^* is the formal adjoint of L.

We are solving the extended system,

$$\begin{cases} Lu = f, & x \in \Omega, \\ \text{suitable b.c. and i.v.}, & x \in \partial\Omega, \\ L^*\phi(y,x) = \delta_y(x), & x \in \Omega, \\ \text{adjoint b.c. and i.v.}, & x \in \partial\Omega. \end{cases}$$

Green's functions

Based on the bilinear identity, we obtain a representation formula for the value of the solution of the original problem at a point $y \in \Omega$,

$$u(y) = (u, \delta_y) = (y, L^* \phi) = (Lu, \phi) = (f, \phi).$$

The imposition of the adjoint boundary conditions is key here.

Green's functions

Example

For

$$\begin{cases} -\Delta u = f, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

ϕ solves

$$\begin{cases} -\Delta \phi(y;x) = \delta_y(x), & x \in \Omega, \\ \phi(y;x) = 0, & x \in \partial\Omega, \end{cases}$$

and the bilinear identity reads

$$u(y) = \int_\Omega f(x)\phi(y;x)\,dx.$$

Green's functions

Green's functions

Example

For

$$\begin{cases} u_t - \Delta u = f, & x \in \Omega, 0 < t \leq T, \\ u(t,x) = 0, & x\partial\Omega, 0 < t \leq T, \\ u(0,x) = 0, & x \in \Omega, \end{cases}$$

ϕ solves

$$\begin{cases} -\phi_t - \Delta\phi = \delta_{(s,y)}(t,x), & x \in \Omega, T > t \geq 0, \\ \phi(t,x) = 0, & x\partial\Omega, T > t \geq 0, \\ \phi(T,x) = 0, & x \in \Omega, \end{cases}$$

and the bilinear identity reads

$$u(s,y) = \int_0^T \int_\Omega f(t,x)\phi(s,y;t,x)\,dxdt.$$

Green's functions

Motivations:

- The Green's function is defined without reference to the particular data f that determines a particular solution. The Green's function depends on the operator and its properties.
- The Green's function generally has special properties arising from the properties of the delta function, such as localized support and symmetry.
- The Green's function gives a "low-dimensional" snapshot of the solution.

Green's functions

Example

The Green's function for the Dirichlet problem for the Laplacian $L = -\Delta$ on the ball Ω of radius r centered at the origin in $\mathbb{R}^3$ is

$$\phi(y;x) = \frac{1}{4\pi} \times \begin{cases} |y-x|^{-1} - r|y|^{-1}\left|\frac{r^2 y}{|y|^2} - x\right|^{-1}, & y \neq 0, \\ |x|^{-1} - r^{-1}, & y = 0, \end{cases}$$

where $|x|$ denotes the Euclidean norm of x

The formula for the disk of radius r is

$$\phi(y;x) = \frac{1}{2\pi} \times \begin{cases} \ln\left(\frac{|y|\left|\frac{r^2 y}{|y|^2} - x\right|}{r|y-x|}\right), & y \neq 0, \\ \ln\left(\frac{r}{|x|}\right), & y = 0. \end{cases}$$

Green's functions

Important issues: Existence, uniqueness, and smoothness of the Green's function.

Generally, everything goes as for the original problem except that the Green's function may not be very smooth or may even be undefined at a point.

The point of evaluation y must lie inside the domain Ω. The Green's function often behaves badly in the limit of y approaching the boundary.

By the way, the theory also extends to over-determined problems.

However, if the original problem is under-determined, this approach fails.

Green's functions

Many expositions of the Green's function avoid the adjoint.

When the original problem has a unique solution and the original operator is the adjoint to the adjoint operator, the Green's function ϕ for the original problem and the Green's function for the adjoint problem ϕ^* are related via

$$\phi(y;x) = \phi^*(x;y).$$

This is known as the reciprocity theorem.

This makes it possible to introduce Green's functions for some kinds of problems without talking about the adjoint.

This depends on the dual space of the dual space of the original space being identifiable with the original space.

Green's functions

Including nonhomogeneous conditions is really a minor issue that usually "solves itself" without trouble.

We carry out the analysis using the Green's function for the homogeneous problem and some additional integrals involving data and the Green's function will appear.

Green's functions

Example
Suppose the problem is

$$\begin{cases} -\Delta u = f, & x \in \Omega, \\ u = g, & x \in \partial\Omega. \end{cases}$$

We define the Green's function as for the homogeneous problem, i.e.,

$$\begin{cases} -\Delta \phi(y;x) = \delta_y(x), & x \in \Omega, \\ \phi(y;x) = 0, & x \in \partial\Omega. \end{cases}$$

Green's functions

Evaluating the bilinear identity yields

$$\int_\Omega (u\Delta\phi - \phi\Delta u)\,dx = \int_{\partial\Omega} \left(u\frac{\partial\phi}{\partial n} - \phi\frac{\partial u}{\partial n} \right)\,ds = \int_{\partial\Omega} u\frac{\partial\phi}{\partial n}\,ds.$$

This yields

$$u(y) = \int_\Omega f(x)\phi(y;x)\,dx - \int_{\partial\Omega} g(s)\frac{\partial\phi(y;s)}{\partial n}\,ds.$$

Green's functions

Different representations are possible.

Example
For

$$\begin{cases} -\Delta u = f, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

We can define the Green's function as the solution of

$$\begin{cases} -\Delta \phi(y;x) = 0, & x \in \Omega, \\ \phi(y;x) = \delta_y(x), & x \in \partial\Omega. \end{cases}$$

Green's functions

Evaluating the bilinear identity yields

$$\int_\Omega (u\Delta\phi - \phi\Delta u)\,dx = \int_{\partial\Omega} \left(u\frac{\partial\phi}{\partial n} - \phi\frac{\partial u}{\partial n} \right)\,ds$$
$$= -\int_{\partial\Omega} \phi\frac{\partial u}{\partial n}\,ds = -\int_{\partial\Omega} \delta_y \frac{\partial u}{\partial n}\,ds = -\frac{\partial u}{\partial n}(y).$$

This gives the value of the normal derivative of u at a point y on the boundary,

$$\frac{\partial u}{\partial n}(y) = -\int_\Omega \phi(y;x) f(x)\,dx.$$

Green's functions

A Posteriori *Error Analysis and Adaptive Error Control*

A generalization of the Green's function

The Green's function yields

$$u(y) = (u, \delta_y) = (\phi(y; x), f(x)).$$

The value of a function at a point is an example of a linear functional.

There are frequently other quantities of interest that can be expressed as functionals.

The Riesz Representation theorem suggests these functionals have the form (u, ψ) for a suitable distribution ψ.

A generalization of the Green's function

Some useful choices of ψ include:

- We can construct $\psi = \delta_c$ to get the average value $\oint_c e(s)\, ds$ of the error over a curve c in $\mathbb{R}^n$, $n = 2, 3$, and $\psi = \delta_s$ to get the average value of the error over a plane surface s in $\mathbb{R}^3$.

A generalization of the Green's function

This choice requires a certain smoothness, which is given by

Theorem
Sobolev If $s > k + n/2$, then there is a constant C such that for $f \in H^s(\mathbb{R}^n)$,

$$\max_{|\alpha| \leq k} \sup_{x \in \mathbb{R}^n} |D^\alpha(x)| \leq C \|f\|_s.$$

This implies that the derivatives of f of order k and less are continuous.

The Sobolev theorem shows that if $k \leq n$ and $s > k/2$, restricting a function in H^s to a submanifold of (co)dimension k is well-defined.

A generalization of the Green's function

Some useful choices of ψ include:

- We can construct $\psi = \delta_c$ to get the average value $\oint_c e(s)\,ds$ of the error over a curve c in $\mathbb{R}^n$, $n = 2, 3$, and $\psi = \delta_s$ to get the average value of the error over a plane surface s in $\mathbb{R}^3$.
- We can obtain errors in derivatives using dipoles in a similar way.
- $\psi = \chi_\omega / |\omega|$ gives the error in the average value over a subset $\omega \subset \Omega$, where χ_ω is the characteristic function of ω.
- Choosing ψ to be the residual of the finite element approximation sometimes yields the energy norm of the error.
- $\psi = \chi_\omega e / \|e\|_\omega$, where e is the error of the finite element discretization, gives the $L^2(\omega)$ norm of the error.

Only some of these data ψ have spatially local support.

A generalization of the Green's function

We consider

$$\begin{cases} Lu = f, & x \in \Omega, \\ \text{suitable b.c. and i.v.}, & x \in \partial\Omega, \end{cases}$$

where L is a linear differential operator.

The boundary and/or initial conditions should insure there is a unique solution.

A generalization of the Green's function

Definition
The **generalized Green's function** corresponding to the quantity of interest (u, ψ) satisfies

$$\begin{cases} L^*\phi(y,x) = \psi(x), & x \in \Omega, \\ \text{adjoint b.c. and i.v.}, & x \in \partial\Omega, \end{cases}$$

where L^* is the formal adjoint of L.

Discretization by the finite element method

We concentrate on

$$\begin{cases} Lu = f, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

where

$$L(D, x)u = -\nabla \cdot a(x)\nabla u + b(x) \cdot \nabla u + c(x)u(x),$$

with $u : \mathbb{R}^n \to \mathbb{R}$, a is a $n \times n$ matrix function of x, b is a n-vector function of x, and c is a function of x.

Discretization by the finite element method

We assume

- $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, is a smooth or polygonal domain
- $a = (a_{ij})$, where $a_{i,j}$ are continuous in $\overline{\Omega}$ for $1 \leq i, j \leq n$ and there is a $a_0 > 0$ such that $v^\top a v \geq a_0$ for all $v \in \mathbb{R}^n \setminus \{0\}$ and $x \in \Omega$
- $b = (b_i)$ where b_i is continuous in $\overline{\Omega}$
- c and f are continuous in $\overline{\Omega}$

Discretization by the finite element method

The associated variational formulation reads

Find $u \in H_0^1(\Omega)$ such that

$A(u,v) = (a\nabla u, \nabla v) + (b \cdot \nabla u, v) + (cu, v) = (f, v)$ for all $v \in H_0^1(\Omega)$.

Discretization by the finite element method

We construct a piecewise polygonal approximation of $\partial\Omega$ whose nodes lie on $\partial\Omega$ and which is contained inside Ω.

This forms the boundary of a convex polygonal domain Ω_h.

$\mathcal{T}_h$ denotes a simplex triangulation of Ω_h that is locally quasi-uniform.

h_K denotes the length of the longest edge of $K \in \mathcal{T}_h$ and h is the mesh function with $h(x) = h_K$ for $x \in K$.

We also use h to denote $\max_K h_K$.

Discretization by the finite element method

Discretization of a domain Ω with curved boundaries.

Discretization by the finite element method

V_h denotes the space of functions that are

- continuous on Ω
- piecewise linear on Ω_h with respect to $\mathcal{T}_h$
- zero on the boundary $\partial\Omega_h$ and $\Omega \setminus \Omega_h$

$V_h \subset H_0^1(\Omega)$, and for smooth functions, the error of interpolation into V_h is $\mathbf{O}(h^2)$ in $\| \ \|$

Definition
The **finite element method** is:

Compute $U \in V_h$ such that $A(U, v) = (f, v)$ for all $v \in V_h$.

An *a posteriori* analysis for an algebraic equation

Estimate the error $e = x - X$ of a numerical solution X of

$$Ax = b$$

where $b, x \in \mathbb{R}^n$ and A is a $n \times n$ matrix.

The computable residual error of X is

$$R = AX - b$$

Goal: Find a relation between the residual and the error.

The residual can be small even if the error is large.

An *a posteriori* analysis for an algebraic equation

Since the residual error of the true solution is zero

$$Ae = -R.$$

To obtain an estimate on a quantity of interest, we introduce the generalized Green's vector solving the adjoint problem

$$A^\top \phi = \psi,$$

where ψ is any unit vector.

This gives an *a posteriori* estimate

$$|(e, \psi)| = |(e, A^\top \phi)| = |(Ae, \phi)| = |(R, \phi)|.$$

An *a posteriori* analysis for an algebraic equation

A posteriori error bound

$$|(e, \psi)| \leq \|\phi\| \, \|R\|.$$

Definition
$\|\phi\|$ is called the **stability factor**

$$\left| \left(\frac{e}{\|x\|}, \psi \right) \right| \leq \text{cond}_{\psi}(A) \, \frac{\|R\|}{\|b\|},$$

where the "weak" condition number is

$$\text{cond}_{\psi}(A) = \|\phi\| \, \|A\| = \|A^{-\top}\psi\| \, \|A\|$$

An *a posteriori* analysis for a finite element method

Goal: Estimate the error in a quantity of interest computed from the finite element solution U.

We use a generalized Green's function ϕ solving the adjoint problem corresponding to a special choice of data ψ.

The error in the desired information may not have much to do with the error in some global norm.

It may be computationally infeasible as well as very inefficient to attempt to control the error in a global norm when all that is desired is accuracy in some quantities of interest.

An *a posteriori* analysis for a finite element method

We assume that the information can be represented as (u, ψ).

Definition
The **generalized Green's function** ϕ solves the **weak adjoint problem** : Find $\phi \in H_0^1(\Omega)$ such that

$$A^*(v, \phi) = (\nabla v, a\nabla\phi) - (v, \text{div}\,(b\phi)) + (v, c\phi) = (v, \psi) \text{ for all } v \in H_0^1(\Omega),$$

corresponding to the adjoint problem $L^*(D, x)\phi = \psi$.

An *a posteriori* analysis for a finite element method

$$
\begin{aligned}
(e,\psi) &= (\nabla e, a\nabla\phi) - (e, \mathsf{div}\,(b\phi)) + (e, c\phi) \\
&= (a\nabla e, \nabla\phi) + (b\cdot\nabla e, \phi) + (ce, \phi) \\
&= (a\nabla u, \nabla\phi) + (b\cdot\nabla u, \phi) + (cu, \phi) \\
&\qquad\qquad - (a\nabla U, \nabla\phi) - (b\cdot\nabla U, \phi) - (cU, \phi) \\
&= (f, \phi) - (a\nabla U, \nabla\phi) - (b\cdot\nabla U, \phi) - (cU, \phi).
\end{aligned}
$$

An *a posteriori* analysis for a finite element method

Definition
$\pi_h \phi$ denotes an approximation of ϕ in V_h

Theorem
The error in the quantity of interest computed from the finite element solution satisfies the **error representation**,

$$(e, \psi) = (f, \phi - \pi_h \phi) - (a \nabla U, \nabla(\phi - \pi_h \phi)) - (b \cdot \nabla U, \phi - \pi_h \phi) - (cU, \phi - \pi_h \phi),$$

where ϕ is the generalized Green's function corresponding to data ψ.

An *a posteriori* analysis for a finite element method

We use the error representation by approximating ϕ using a relatively high order finite element method.

Good results are obtained using the space V_h^2

Definition
The **approximate generalized Green's function** satisfies:
Compute $\Phi \in V_h^2$ such that

$$A^*(v,\Phi) = (\nabla v, a\nabla\Phi) - (v, \text{div}\,(b\Phi)) + (v, c\Phi) = (v,\psi) \text{ for all } v \in V_h^2.$$

The **approximate error representation** is

$$(e,\psi) \approx (f, \Phi - \pi_h\Phi) - (a\nabla U, \nabla(\Phi - \pi_h\Phi)) \\ - (b\cdot\nabla U, \Phi - \pi_h\Phi) - (cU, \Phi - \pi_h\Phi).$$

An *a posteriori* analysis for a finite element method

Examples are computed using FETkLab.

- Runs under *MATLAB*
- Solves general nonlinear elliptic systems on general domains in two space dimensions
- Implements the *a posteriori* error estimate for 16 simultaneous adjoint data ψ_i
- Uses bisection or red-green quadrisection to refine elements
- Only those elements whose element indicators are larger than the mean plus one standard deviation of all of the element indicators in that level are refined.

An *a posteriori* analysis for a finite element method

Example

An elliptic problem on the unit square $\Omega = (0,1) \times (0,1)$

$$\begin{cases} -\Delta u = 200 \sin(10\pi x) \sin(10\pi y), & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega \end{cases}$$

The solution is highly oscillatory

$$u(x,y) = \sin(10\pi x) \sin(10\pi y).$$

An *a posteriori* analysis for a finite element method

Highly oscillatory solution.

An *a posteriori* analysis for a finite element method

We estimate the error in the average value by choosing $\psi \equiv 1$.

The generalized Green's function is approximated on the same mesh using a piecewise quadratic finite element function.

We plot the ratios error/estimate for a wide variety of meshes.

An *a posteriori* analysis for a finite element method

Plots of the error/estimate ratio.

Adaptive error control

Goal of adaptive error control: Generate a mesh with a relatively small number of elements such that for a given tolerance TOL and data ψ,

$$|(e, \psi)| \leq \text{TOL}.$$

This cannot be verified in practice.

Adaptive error control

Rewrite the error representation elementwise:

$$(e,\psi) \approx \sum_{K\in\mathcal{T}_h} \int_K \big((f - b\cdot\nabla U - cU)(\Phi - \pi_h\Phi) - a\nabla U\cdot\nabla(\Phi - \pi_h\Phi)\big)\,dx.$$

Definition
The **mesh acceptance criterion** is

$$\left|\sum_{K\in\mathcal{T}_h} \int_K \big((f - b\cdot\nabla U - cU)(\Phi - \pi_h\Phi) - a\nabla U\cdot\nabla(\Phi - \pi_h\Phi)\big)\,dx\right| \leq \text{TOL}$$

If this is satisfied, then the numerical solution is deemed acceptable.

Adaptive error control

When the mesh criterion is not satisfied, we have to “enrich” the discretization.

The cancellation among the contributions from each element make the enrichment decision problematic.

There is currently no theory or practical method for accommodating cancellation of errors in an adaptive error control in a way that achieves true optimality of efficiency.

Adaptive error control

A standard approach is to formulate the discretization selection problem as an optimization problem.

This requires an estimate consisting of a sum over elements of positive quantities.

Inserting norms gives

$$|(e,\psi)| \leq \sum_{K\in\mathcal{T}_h} \int_K \left|(f-b\cdot\nabla U-cU)(\Phi-\pi_h\Phi)-a\nabla U\cdot\nabla(\Phi-\pi_h\Phi)\right| dx.$$

If the acceptance criterion fails, the mesh is refined to achieve

$$\sum_{K\in\mathcal{T}_h} \int_K \left|(f-b\cdot\nabla U-cU)(\Phi-\pi_h\Phi)-a\nabla U\cdot\nabla(\Phi-\pi_h\Phi)\right| dx \leq \text{TOL}.$$

Adaptive error control

The calculus of variations yields
"Principle of Equidistribution" The element contributions on a nearly optimal mesh are roughly equal across the elements.

Definition
Two **element acceptance criteria** for the **element indicators** are

$$\max_K \left|(f - b\cdot\nabla U - cU)(\Phi - \pi_h\Phi) - a\nabla U\cdot\nabla(\Phi - \pi_h\Phi)\right| \lesssim \frac{\mathrm{TOL}}{|\Omega|},$$

or

$$\int_K \left|(f - b\cdot\nabla U - cU)(\Phi - \pi_h\Phi) - a\nabla U\cdot\nabla(\Phi - \pi_h\Phi)\right| dx \lesssim \frac{\mathrm{TOL}}{M},$$

where M is the number of elements in $\mathcal{T}_h$.

Adaptive error control

Computing a mesh using these criteria is usually performed by a “compute-estimate-mark-refine” adaptive strategy.

We start with a coarse mesh then successively refine some fraction of the elements on which the element acceptance criterion fails.

Adaptive error control

Example

$$\begin{cases} -\Delta u = \\ \qquad \frac{4800}{\pi}\big(1 - 400((x-.5)^2 + (y-.5)^2)\big)e^{-400((x-.5)^2+(y-.5)^2)}, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (x,y) \in \Omega, \\ u(x,y) = 0, \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (x,y) \in \partial\Omega, \end{cases}$$

f is an approximation of a delta function at $(.5, .5)$.

We control the error in the average value using a tolerance of $.05\%$.

Adaptive error control

Results for the initial mesh.

Adaptive error control

Results after 10 iterations.

Adaptive error control

The error/estimate ratio.

Further analysis on the *a posteriori* error estimate

We derive a more common form of the estimate for the simple problem with $L(u) = -\Delta u$.

The error representation formula is

$$(e, \psi) = \int_\Omega f(\phi - \pi_h \phi)\, dx - \int_\Omega \nabla U \cdot \nabla(\phi - \pi_h \phi)\, dx.$$

We break up the second integral on the right as

$$\int_\Omega \nabla U \cdot \nabla(\phi - \pi_h \phi)\, dx = \sum_{K \in \mathcal{T}_h} \int_K \nabla U \cdot \nabla(\phi - \pi_h \phi)\, dx.$$

Further analysis on the *a posteriori* error estimate

Using Green's formula,

$$\int_K \nabla U \cdot \nabla(\phi - \pi_h \phi)\, dx = -\int_K \Delta U(\phi - \pi_h \phi)\, dx + \int_{\partial K} \nabla U \cdot n_{\partial K}(\phi - \pi_h \phi)\, ds,$$

where the last term is a line integral and $n_{\partial K}$ denotes the outward normal to ∂K.

Summing over all of the elements, the boundary integrals give two contributions from each element edge, computed in opposite directions.

Further analysis on the *a posteriori* error estimate

If $K_1, K_2 \in \mathcal{T}_h$ share a common edge $\sigma_1 \subset \partial K_1 = \sigma_2 \subset \partial K_2$, then

$$\begin{aligned}
\int_{\sigma_1} \nabla U|_{K_1} \cdot n_{\sigma_1}(\phi - \pi_h\phi)\, ds + \int_{\sigma_2} \nabla U|_{K_2} \cdot n_{\sigma_2}(\phi - \pi_h\phi)\, ds \\
&= \int_{\sigma_1} \nabla U|_{K_1} \cdot n_{\sigma_1}(\phi - \pi_h\phi)\, ds \\
&\qquad - \int_{\sigma_1} \nabla U|_{K_2} \cdot n_{\sigma_1}(\phi - \pi_h\phi)\, ds \\
&= -\int_{\sigma_1} [\nabla U] \cdot n_{\sigma_1}(\phi - \pi_h\phi)\, ds,
\end{aligned}$$

where $[U] = \nabla U|_{K_2} - \nabla U|_{K_1}$ denotes the "jump" in ∇U across σ_1 in the direction of the normal $n_{\partial K_1}$.

Further analysis on the *a posteriori* error estimate

An alternate error representation,:

$$(e,\psi) = -\sum_{K\in\mathcal{T}_h}\left(\int_K (\Delta U + f)(\phi - \pi_h\phi)\,dx \right.$$
$$\left. -\frac{1}{2}\int_{\partial K}[\nabla U]\cdot n_{\partial K}(\phi - \pi_h\phi)\,ds\right).$$

Further analysis on the *a posteriori* error estimate

Definition

The **residual** and corresponding **adjoint** or **dual weights** are

$$\mathcal{R}_K = \begin{pmatrix} \|\Delta U + f\|_K \\ \|h^{-1/2}[\nabla U]\|_{\partial K}/2 \end{pmatrix}, \ \mathcal{W}_K = \begin{pmatrix} \|\phi - \pi_h \phi\|_K \\ \|h^{1/2}(\phi - \pi_h \phi)\|_{\partial K} \end{pmatrix}.$$

Theorem

The error of the finite element approximation is bounded by

$$|(e, \psi)| \leq \sum_{K \in \mathcal{T}_h} \mathcal{R}_K \cdot \mathcal{W}_K.$$

Further analysis on the *a posteriori* error estimate

We derive *a priori* bounds on the residual and dual weights.

There is a constant C independent of the mesh such that

$$\mathcal{R}_K \leq C|K|^{1/2},$$

where $|K|$ denote the area of $K \in \mathcal{T}_h$.

The bound on the first component follows from
$\|\Delta U + f\|_K = \|f\|_K \leq \max_\Omega |f| \times |K|^{1/2}$.

Further analysis on the *a posteriori* error estimate

For the second component, consider an integral over the common edge σ between two elements K_1 and K_2,

$$\|[\nabla U]\|_\sigma = \|\nabla U|_{K_2} - \nabla U|_{K_1}\|_\sigma \leq \|\nabla U|_{K_2} - \nabla u|_\sigma\|_\sigma + \|\nabla u|_\sigma - \nabla U|_{K_1}\|_\sigma.$$

By a trace inequality, the standard energy norm convergence result, and a standard elliptic regularity result,

$$\begin{aligned}\|\nabla U|_{K_i} - \nabla u|_\sigma\|_\sigma &\leq \|\nabla U - \nabla u\|_{K_i}^{1/2} \|\nabla U - \nabla u\|_{1,K_i}^{1/2} \\ &\leq C\|hu\|_{2,K_i}^{1/2} \|u\|_{2,K_i}^{1/2} \\ &\leq C\|h^{1/2} f\|_{K_i},\end{aligned}$$

for $i = 1, 2$. The local quasi-uniformity of the mesh implies

$$\frac{1}{2}\|h^{-1/2}[\nabla U]\|_{\partial K} \leq C \max_\Omega |f| \times |K|^{1/2}.$$

Further analysis on the *a posteriori* error estimate

Clearly, the convergence of the Galerkin approximation is strongly influenced by the dual weights $\phi - \pi_h \phi$, i.e. by the approximation properties of V_h and the smoothness of ϕ.

This reflects the importance of the cancellation of errors inherent to the Galerkin method.

The Effective Domain of Influence and Solution Decomposition

The Effective Domain of Influence

A characteristic property of elliptic partial differential equations is a global domain of influence.

A local perturbation of data near one point affects the solution throughout the domain of the problem.

Elliptic problems also have the property that the strength of the effect of a localized perturbation on a solution decays significantly with the distance from the support of the perturbation, at least in some directions.

It turns out that this property also has profound consequences for the numerical solution of elliptic problems.

The Effective Domain of Influence

Example
Consider the Green's function for the Dirichlet problem for the Laplacian $-\Delta u = f$ on the ball Ω of radius r centered at the origin in $\mathbb{R}^3$.

If the data f is perturbed by a smooth function δf, the perturbation in the value of the solution $\delta u(y)$ is given by

$$\delta u(y) = \int_\Omega \phi(y;x)\delta f(x)\,dx, \quad y \in \Omega.$$

The Effective Domain of Influence

If δf has compact support $\text{supp}(\delta f) \subset \Omega$,

$$|y - x| \leq \left| \frac{r^2 y}{|y|^2} - x \right|, \quad x \in \text{supp}(\delta f),\ y \in \Omega \setminus \text{supp}(\delta f).$$

We conclude that

$$|\delta u(y)| \leq \frac{\max |\delta f| \ \times \ \text{volume of } \text{supp}(\delta f) \times \left(1 + \frac{r}{|y|}\right)}{4\pi \times \text{the distance from } y \text{ to } \text{supp}(\delta f)}.$$

Poisson's equation in a disk

Ω denotes the disk of radius r centered at the origin in $\mathbb{R}^2$

Consider the Dirichlet problem for the Laplacian $L = -\Delta u = f$.

Suppose that ω is a small region contained in Ω located well away from $\partial\Omega$.

We wish to estimate the error $e = u - U$ in the energy norm $\|e\|_{1,\omega}$ in ω.

Poisson's equation in a disk

Poisson's equation in a disk

We evaluate the norm weakly

$$\|e\|_{1,\omega} = \sup_{\substack{\psi \in H^{-1}(\omega) \\ \|\psi\|_{-1,\omega}=1}} (e, \psi).$$

The supremum is achieved for some $\psi \in H^{-1}(\omega)$.

We extend ψ to $H^{-1}(\Omega)$ by setting it to zero in $\Omega \setminus \omega$.

To discuss orders of convergence, we use the *a posteriori* bound.

Poisson's equation in a disk

$G(x;y)$ denotes the Green's function for the Laplacian on Ω, so

$$\phi(x) = \int_\Omega G(x;y)\psi(y)\,dy = \int_\omega G(x;y)\psi(y)\,dy.$$

Recall,

$$G(x;y) = \frac{1}{2\pi} \times \begin{cases} \ln\left(\dfrac{|x|\left|\frac{r^2 x}{|x|^2} - y\right|}{r|x-y|}\right), & x \neq 0, \\ \ln\left(\frac{r}{|y|}\right), & x = 0. \end{cases}$$

Poisson's equation in a disk

Case 1: For $y \in \omega$, $G(x;y)$ is a smooth function of x for $x \in \Omega \setminus \omega$ and so is ϕ.

We assume that $\delta > 0$ satisfies

- It is small enough that $\omega_\delta = \{x \in \Omega : \text{dist}\,(x, \omega) \leq \delta\}$ is contained in Ω
- It is large enough that for $K \subset \Omega \setminus \omega_\delta$, the union $\mathcal{N}(K)$ of K and the elements bordering K does not intersect ω

Poisson's equation in a disk

For $K \subset \Omega \setminus \omega_\delta$, we let π_h be the Lagrange nodal interpolant with respect to $\mathcal{T}_h$, so that

$$\|\phi - \pi_h\phi\|_K \leq C \sum_{|\alpha|=2} \|h^2 D^\alpha \phi\|_K.$$

Poisson's equation in a disk

Case 2: ϕ is not so smooth in ω.

For $K \cap \omega_\delta \neq \emptyset$, π_h is the Scott-Zhang interpolant, for which

$$\|\phi - \pi_h \phi\|_K \leq C |h\phi|_{1,\mathcal{N}(K)},$$

for a mesh-independent constant C.

Poisson's equation in a disk

The second component of $\mathcal{W}_K$ is bounded similarly after using a trace theorem,

$$\|h^{1/2}(\phi - \pi_h\phi)\|_{\partial K} \leq \|\phi - \pi_h\phi\|^{1/2}_{\mathcal{N}(K)} \|h(\phi - \pi_h\phi)\|^{1/2}_{1,\mathcal{N}(K)},$$

and the local quasi-uniformity of the mesh.

Poisson's equation in a disk

We conclude,

Theorem

For any $\delta > 0$ small enough that $\omega_\delta \subset \Omega$ but large enough that $\mathcal{N}(K) \cap \omega = \emptyset$ for $K \subset \Omega \setminus \omega_\delta$, there is a constant C such that

$$\|e\|_{1,\omega} \leq \sum_{K \subset \Omega \setminus \omega_\delta} \sum_{|\alpha|=2} C \|h^2 D^\alpha \phi\|_K |K|^{1/2} + \sum_{K \cap \omega_\delta \neq \emptyset} C |h\phi|_{1,\mathcal{N}(K)} |K|^{1/2}.$$

Poisson's equation in a disk

We estimate the quantities in the *a posteriori* bound.

To handle the first sum, we use

$$\begin{aligned}
\|D_x^\alpha \phi\|_K^2 &= \int_K \left(\int_\omega D_x^\alpha G(x,y)\psi(y)\,dy \right)^2 dx \\
&\le \int_K \|D_x^\alpha G(x,\cdot)\|_{1,\omega}^2 \|\psi\|_{-1,\omega}^2 \,dx \\
&= \sum_{|\beta|=1} \int_K \int_\omega |D_x^\alpha D_y^\beta G(x,y)|^2 \,dydx + \int_K \int_\omega |D_x^\alpha G(x,y)|^2 \,dydx.
\end{aligned}$$

Poisson's equation in a disk

There is a constant C such that

$$|D_x^\alpha D_y^\beta G(x,y)| \leq \frac{C}{|x-y|^2}, \quad x \neq y \in \Omega,\ |\alpha| = 2,\ |\beta| \leq 1.$$

We conclude there is a constant C independent of the mesh such that for $K \subset \Omega \setminus \omega_\delta$,

$$\|\phi - \pi_h \phi\|_K \leq \frac{C h_K^2}{\text{dist}\,(K,\omega)^2} |K|^{1/2}.$$

Poisson's equation in a disk

To handle the second sum on the right, we use the basic stability estimate,

$$\|\phi\|_{1,\Omega} \leq \|\psi\|_{-1,\Omega} = \|\psi\|_{-1,\omega} = 1.$$

If we assume a uniform (small) size $h_K = \underline{h}$ for elements such that $K \cap \omega_\delta \neq \emptyset$, we obtain

$$\sum_{K \cap \omega_\delta \neq \emptyset} C h_K |\phi|_{1,\mathcal{N}(K)} \leq C\underline{h}\|\phi\|_{1,\Omega} = C\underline{h} \leq \frac{C}{|\omega_\delta|} \sum_{K \cap \omega_\delta \neq \emptyset} \underline{h}|K|.$$

Poisson's equation in a disk

We conclude

Theorem

For any $\delta > 0$ small enough that $\omega_\delta \subset \Omega$ but large enough that $\mathcal{N}(K) \cap \omega = \emptyset$ for $K \subset \Omega \setminus \omega_\delta$, there is a constant C such that

$$\|e\|_{1,\omega} \leq \sum_{K \subset \Omega \setminus \omega_\delta} \frac{C h_K^2}{\text{dist}\,(K, \omega)^2} |K| + \sum_{K \cap \omega_\delta \neq \emptyset} C \underline{h} |K|.$$

Poisson's equation in a disk

We apply the "Principle of Equidistribution"

The element indicators are $Ch_K^2/\text{dist}\,(K,\omega)^2$ respectively $C\underline{h}$, and in an optimal mesh,

$$\frac{h_K^2}{\text{dist}\,(K,\omega)^2} \approx \underline{h} \quad \text{or} \quad h_K \approx \underline{h}^{1/2} \times \text{dist}\,(K,\omega), \qquad K \subset \Omega \setminus \omega_\delta.$$

Poisson's equation in a disk

The decay of influence inherent to the Laplacian on the disk means that away from the region ω where we estimate the norm, we can choose elements asymptotically larger than the element size used in ω_δ.

Moreover, the elements can increase in size as the distance to ω_δ increases

ω_δ is an the effective domain of influence for the error in the energy norm in ω.

Poisson's equation in a disk

Definition
An **effective domain of influence** corresponding to the data ψ is the region ω_ψ in which the corresponding elements must be significantly smaller in size than the elements used in the complement $\Omega \setminus \omega_\psi$ in order to satisfy the adaptive goal.

Equivalently, if $\mathcal{T}_h$ comprises uniformly sized elements, then the effective domain of influence comprises those elements on which the element indicators, are substantially larger than those in the complement.

A decomposition of the solution

Often, the goal of solving a differential equation is to compute several pieces of information.

The problem of computing multiple quantities of interest also arises naturally when the data ψ for the adjoint problem does not have spatially localized support (averages and norms).

We cannot expect a significant localization effect from the decay of influence when the support of the data for the adjoint problem is not spatially localized.

If the data ψ has the property that the adjoint weight $\phi - \pi_h \phi$ has a more-or-less uniform size throughout Ω, then the degree of non-uniformity in an adapted mesh depends largely on the spatial variation of the residual.

A decomposition of the solution

We use a partition of unity to "localize" a problem in which supp (ψ) does not have local support.

Definition
Suppose that $\{\Omega_i\}_{i=1}^N$ is a finite open cover of Ω. A **Lipschitz partition of unity** subordinate to $\{\Omega_i\}$ is a collection of functions $\{p_i\}_{i=1}^N$ with the properties

$$\text{supp}\,(p_i) \subset \overline{\Omega}_i, \quad 1 \le i \le N, \quad \sum_{i=1}^N p_i(x) = 1, \quad x \in \Omega,$$

$$p_i \text{ is continuous on } \Omega \text{ and differentiable on } \Omega_i, \quad 1 \le i \le N,$$

$$\|p_i\|_{L^\infty(\Omega)} \le C \text{ and } \|\nabla p_i\|_{L^\infty(\Omega_i)} \le C/\text{diam}\,(\Omega_i), \quad 1 \le i \le N,$$

where C is a constant and diam (Ω_i) is the diameter of Ω_i.

A decomposition of the solution

Corresponding to a partition of unity $\{p_i\}$, $\psi \equiv \sum_{i=1}^{N} \psi p_i$,

Definition
The quantities $\{(U, \psi p_i)\}$ corresponding to the data $\{\psi_i = \psi p_i\}$ are called the **localized information** corresponding to the partition of unity.

We consider the problem of estimating the error in the localized information for $1 \leq i \leq N$.

A decomposition of the solution

We obtain a finite element solution via:

$$\text{Compute } \hat{U}_i \in \hat{V}_i \text{ such that } A(\hat{U}_i, v) = (f, v) \text{ for all } v \in \hat{V}_i,$$

where $\hat{V}_i$ is a space of continuous, piecewise linear functions on a locally quasi-uniform simplex triangulation $\mathcal{T}_i$ of Ω obtained by local refinement of an initial coarse triangulation $\mathcal{T}_0$ of Ω.

$\{\hat{V}_i\}$ is globally defined and the "localized" problem is solved over the entire domain

We hope that this will require a locally refined mesh because the corresponding data has localized support.

A decomposition of the solution

A partition of unity approximation in the sense of Babuška and Melenk uses $U_i = \chi_i \hat{U}_i$, $1 \leq i \leq N$, where χ_i is the characteristic function of Ω_i.

The local approximation U_i is in the local finite element space $V_i = \chi_i \hat{V}_i$.

Definition
The **partition of unity approximation** is defined by $U_p = \sum_{i=1}^{N} U_i p_i$, which is in the **partition of unity finite element space**

$$V_p = \sum_{i=1}^{N} V_i p_i = \left\{ \sum_{i=1}^{N} v_i p_i : v_i \in V_i \right\}.$$

A decomposition of the solution

The partition of unity approximation recovers the full convergence properties of an approximation of the original solution.

Note

$$U_p = \sum_{i=1}^{N} U_i p_i = \sum_{i=1}^{N} \chi_i \hat{U}_i p_i \equiv \sum_{i=1}^{N} \hat{U}_i p_i.$$

The values of U_i or $\hat{U}_i$ outside of Ω_i are immaterial in forming the global partition of unity approximation.

A decomposition of the solution

We use the generalized Green's function satisfying the adjoint problem:

Find $\phi_i \in H_0^1(\Omega)$ such that $A^*(v, \phi_i) = (v, \psi_i)$ for all $v \in H_0^1(\Omega)$.

We expand the global error

$$(u - U_p, \psi) = \sum_{i=1}^{N} \big((u - U_i)p_i, \psi\big).$$

We estimate each summand on the right as

$$\begin{aligned}\big((u - U_i)p_i, \psi\big) &= (u - \hat{U}_i, \psi_i) = A^*(u - \hat{U}_i, \phi_i) \\ &= (f, \phi_i) - (a\nabla\hat{U}_i, \nabla\phi_i) - (b \cdot \nabla\hat{U}_i, \phi_i) - (c\hat{U}_i, \phi_i).\end{aligned}$$

A decomposition of the solution

Letting $\pi_i \phi_i$ denote an approximation of ϕ_i in $\hat{V}_i$,

Theorem
The error of the partition of unity finite element solution U_p satisfies the error representation,

$$(u - U_p, \psi) = \sum_{i=1}^{N} \Big((f, \phi_i - \pi_i \phi_i) - (a \nabla \hat{U}_i, \nabla(\phi_i - \pi_i \phi_i)) - (b \cdot \nabla \hat{U}_i, \phi_i - \pi_i \phi_i) - (c \hat{U}_i, \phi_i - \pi_i \phi_i) \Big).$$

A decomposition of the solution

Definition
The **approximate generalized Green's functions** solve:
Compute $\Phi_i \in V_i^2$ such that

$$A^*(v, \Phi_i) = (v, \psi_i) \text{ for all } v \in V_i^2, \quad 1 \le i \le N,$$

where V_i^2 is the space of continuous, piecewise quadratic functions with respect to $\mathcal{T}_i$.

The **approximate error representations** are

$$(u - \hat{U}_i, \psi_i) \approx (f, \Phi_i - \pi_i \Phi_i) - (a \nabla \hat{U}_i, \nabla(\Phi_i - \pi_i \Phi_i))$$
$$- (b \cdot \nabla \hat{U}_i, \Phi_i - \pi_i \Phi_i) - (c \hat{U}_i, \Phi_i - \pi_i \Phi_i).$$

A decomposition of the solution

If the localized error satisfies

$$\left|\left(u - \hat{U}_i, \psi_i\right)\right| \leq \frac{\text{TOL}}{N}, \quad 1 \leq i \leq N,$$

then $|(u - U_p, \psi)| \leq$ TOL.

This justifies treating the N "localized" problems independently in terms of mesh refinement.

Computation of multiple quantities of interest

We present an algorithm for computing multiple quantities of interest efficiently using knowledge of the effective domains of influence of the corresponding Green's functions.

We assume that the information is specified as $\{(U, \psi_i)\}_{i=1}^N$ for a set of N functions $\{\psi_i\}_{i=1}^N$.

These data might arise as particular goals or via localization through a partition of unity.

We assume that the goal is to compute the information associated to ψ_i so that the error is smaller than a tolerance TOL$_i$ for $1 \leq i \leq N$.

Computation of multiple quantities of interest

Two approaches:

Approach 1: **A Global Computation**
Find one triangulation such that the corresponding finite element solution satisfies $|(e, \psi_i)| \leq$ TOL$_i$, for $1 \leq i \leq N$.

Approach 2: **A Decomposed Computation**
Find N independent triangulations and finite element solutions U_i so that the errors satisfy $|(e_i, \psi_i)| \leq$ TOL$_i$, for $1 \leq i \leq N$.

The Global Computation can be implemented with a straightforward modification of the standard adaptive strategy in which the N corresponding mesh acceptance criteria are checked on each element and if any of the N criteria fail, the element is marked for refinement.

Computation of multiple quantities of interest

If the correlation, i.e., overlap, between the effective domains of influence associated to the N data $\{\psi_i\}$ is relatively small and the effective domains of influence are relatively small subsets of Ω, then each individual solution in the Decomposed Computation will require significantly fewer elements than the solution in the Global Computation to achieve the desired accuracy.

This can yield significant computational advantage in terms of lowering the maximum memory requirement to solve the problem.

Computation of multiple quantities of interest

Decreasing the maximum memory required to solve a problem can be significant in at least two situations.

- If the individual solutions in the Decomposed Computation are computed in parallel and they require significantly fewer elements than the Global Computation, we can expect to see significant speedup.
- In an environment with limited memory capabilities, decomposing a Global Computation requiring a large number of elements into a set of significantly smaller computations can greatly increase the accuracy that can be achieved and/or decrease the time required.

Computation of multiple quantities of interest

If the effective domains of influence associated to the N data $\{\psi\}$ have relatively large intersections, then the individual solutions in the Decomposed Computation will require roughly the same number of elements as the solution for the Global Computation.

In this case, there is little to be gained in using the Decomposed Computation.

Computation of multiple quantities of interest

In general, some of the N effective domains of influence associated to data $\{\psi_i\}$ in the Decomposed Computation will correlate significantly and the rest will have low correlation.

We can optimize the use of resources by combining computations for data whose associated domains of influence have significant correlation and treating the rest independently.

Computation of multiple quantities of interest

Determining the Solution Decomposition

1. Discretize Ω by an initial coarse triangulation $\mathcal{T}_0$ and compute an initial finite element solution U_0.
2. Estimate the error in each quantity (U_0, ψ_i) by solving the N approximate adjoint problems and computing the estimate.
3. Using the element indicators associated to identify the effective domains of influence for the data $\{\psi_i\}$ in terms of the mesh $\mathcal{T}_0$ and significant correlations between the effective domains of influence.
4. Decide on the number of approximate solutions to be computed and the subset of information to be computed from each solution.
5. Compute the approximate solutions independently using adaptive error control aimed at computing the specified quantity or quantities of interest accurately.

Identifying significant correlations

The key issue in the proposed algorithm is identifying the effective domains of influence and recognizing significant correlation, or overlap, between different effective domains of influence.

Mesh refinement decisions are based on the sizes of the element indicators

$$\mathcal{E}_i|_K = \max_K \left|(f - b\cdot\nabla\hat{U}_i - c\hat{U}_i)(\Phi_i - \pi_i\Phi_i) - a\nabla\hat{U}_i\cdot\nabla(\Phi_i - \pi_i\Phi_i)\right|$$

or

$$\mathcal{E}_i|_K = \int_K \left|(f - b\cdot\nabla\hat{U}_i - c\hat{U}_i)(\Phi_i - \pi_i\Phi_i) - a\nabla\hat{U}_i\cdot\nabla(\Phi_i - \pi_i\Phi_i)\right| dx,$$

Identifying significant correlations

Definition
We let $\mathcal{E}_i(x)$ denote the piecewise constant **element error indicator function** associated to data ψ_i with $\mathcal{E}_i(x) \equiv \mathcal{E}_i|_K$ for $K \in \mathcal{T}_0$.

Identifying the effective domain of influence means finding a set of elements on which the element error indicators are significantly larger than on the complement.

Identifying significant correlation between the effective domains of influence of two data entails showing that the effective domains of influence have a significant number of elements in common.

Identifying significant correlations

Pattern matching uses

Definition
The **(cross-)correlation** of two functions $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$, defined as:

$$(f \circ g)(y) = \int_\Omega f(x) g(y+x)\, dx,$$

which is an $L^1(\Omega)$ function.

The **correlation indicator** $c(f, g)$ is a functional of the correlation function $(f \circ g)$.

We treat the element error indicator functions $\{\mathcal{E}_i\}$ as signal functions.

Identifying significant correlations

Discounting translation or rotation, correlation of $\mathcal{E}_i$ and $\mathcal{E}_j$ reduces to the L^2-inner-product:

$$(\mathcal{E}_i \circ \mathcal{E}_j)(0) = \int_\Omega \mathcal{E}_i(x)\mathcal{E}_j(x)\,dx = (\mathcal{E}_i, \mathcal{E}_j)_\Omega.$$

Definition
The **correlation indicator** $c(\mathcal{E}_i, \mathcal{E}_j)$ is

$$c(\mathcal{E}_i, \mathcal{E}_j) = |(\mathcal{E}_i \circ \mathcal{E}_j)(0)| = (\mathcal{E}_i, \mathcal{E}_j)_\Omega.$$

Identifying significant correlations

Definition
We say that the effective domain of influence associated to ψ_i is **significantly correlated** to the domain of influence associated to ψ_j if two conditions hold.

Identifying significant correlations

Definition
We say that the effective domain of influence associated to ψ_i is **significantly correlated** to the domain of influence associated to ψ_j if two conditions hold.

Condition 1
The correlation of $\mathcal{E}_i$ and $\mathcal{E}_j$ is larger than a fixed fraction of the norm of $\mathcal{E}_j$, or

$$\text{Correlation Ratio 1} = \frac{c(\mathcal{E}_i, \mathcal{E}_j)}{\|\mathcal{E}_j\|^2} \geq \gamma_1,$$

for some fixed $0 \leq \gamma_1 \leq 1$.

This means that the projection of $\mathcal{E}_i$ onto $\mathcal{E}_j$ is sufficiently large.

Identifying significant correlations

Three examples of significant correlation of $\mathcal{E}_i$ with $\mathcal{E}_j$. Plotted are the element indicator functions $\mathcal{E}_i(x), \mathcal{E}_j(x)$ versus the element number.

Identifying significant correlations

Definition
We say that the effective domain of influence associated to ψ_i is **significantly correlated** to the domain of influence associated to ψ_j if two conditions hold.

Condition 2
The component of $\mathcal{E}_j$ orthogonal to $\mathcal{E}_i$ is smaller than a fixed fraction of the norm of $\mathcal{E}_j$, or

$$\text{Correlation Ratio 2} = \frac{\left\| \mathcal{E}_j - \frac{c(\mathcal{E}_j, \mathcal{E}_i)}{\|\mathcal{E}_i\|^2} \mathcal{E}_i \right\|}{\|\mathcal{E}_j\|} \leq \gamma_2,$$

for some fixed $0 \leq \gamma_2 \leq 1$.

This corrects for the difficulties that arise when $\mathcal{E}_i$ is much larger than $\mathcal{E}_j$.

Identifying significant correlations

An example in which the second condition fails.

Identifying significant correlations

Plots of nine element indicator functions $\mathcal{E}_i$ versus the element number.

Identifying significant correlations

With $\gamma_1 = .9$ and $\gamma_2 = .7$:

$\mathcal{E}_1$ with $\mathcal{E}_8$	$\mathcal{E}_4$ with none	$\mathcal{E}_7$ with none
$\mathcal{E}_2$ with $\mathcal{E}_6, \mathcal{E}_7$	$\mathcal{E}_5$ with $\mathcal{E}_2, \mathcal{E}_6$	$\mathcal{E}_8$ with none
$\mathcal{E}_3$ with $\mathcal{E}_1, \mathcal{E}_8$	$\mathcal{E}_6$ with none	$\mathcal{E}_9$ with none

We emphasize that the initial identification of significant correlation between effective domains of influence of various Green's functions in a computation is carried out on a coarse initial partition of the domain and hence is relatively inexpensive.

Examples

We solve elliptic problems using adaptive mesh refinement to achieve accuracy in a set of quantities of interest using a Global Computation and a Decomposed Computation.

The results suggest that the individual solutions in the Decomposed Computation require significantly fewer elements to achieve the desired accuracy than the Global Computation in a variety of situations.

Examples

As a relatively universal measure of the gain from using the Decomposed Computation, we use

Definition
The **Final Element Ratio** is the number of elements in the final mesh refinement level required to achieve accuracy in the specified quantities of interest in the Global Computation to the maximum number of elements in the final mesh refinement levels for the individual computations in the Decomposed Computation.

Generally, we expect the gain in efficiency to scale super-linearly with the Final Element Ratio.

We compute the Final Element Ratio using solutions that are have roughly the same accuracy.

Examples

Example 1

We solve

$$\begin{cases} -\frac{1}{10\pi^2}\Delta u(x) = \sin(\pi x)\sin(\pi y), & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega, \end{cases}$$

on the $\Omega = [0,8] \times [0,8]$.

The solution is $u(x,y) = 5\sin(\pi x)\sin(\pi y)$.

Goal: Control the error in the average value of u by choosing $\psi \equiv 1/|\Omega| = 1/64$.

Examples

Global Computation: Mesh is adapted the error in the average value of u is smaller than the error tolerance of 5%.

Initial mesh is 10×10 elements and after five refinement levels, we end up with 3505 elements, achieving an error of $.022$.

Examples

Initial and final meshes.

Examples

Numerical solutions.

Examples

Estimates, errors, and error/estimate ratios:

Level	Elements	Estimate	Error	Ratio
1	100	.1567	.1534	.9786
2	211	.1157	.1224	1.058
3	585	.3063	.3078	1.005
4	1309	.1159	.1166	1.006
5	3505	.02163	.02148	.9975

Examples

6	7	10	11
5	8	9	12
2	3	14	15
1	4	13	16

Partitions for the decomposition.

Examples

The partition of unity yields four data $\{\psi_1, \psi_2, \psi_3, \psi_4\}$.

We compute the four localized approximations $\{\hat{U}_1, \cdots, \hat{U}_4\}$ using the same initial mesh as before.

The Correlation Ratios indicates that all four localized solutions should be computed independently.

Examples

We obtain acceptable results using the tolerance of 5%.

Data	Level	Elements	Estimate
ψ_1	3	618	$.01242$
ψ_2	3	575	$-.0009109$
ψ_3	3	618	$.01242$
ψ_4	3	575	$-.0009109$

This yields a partition of unity solution U_p with accuracy $.023$.

Using the Decomposed Computation yields a Final Element Ratio of ≈ 5.7.

Examples

Final Mesh for $\widehat{U}_1$

Final Mesh for $\widehat{U}_2$

Two of the final meshes.

Examples

The generalized Green's functions for the global average error and the localized data ψ_2.

Examples

A Decomposed Computation using a partition of unity on 16 equal-sized regions yields significant correlations:

$\mathcal{E}_2$ with $\mathcal{E}_3$	$\mathcal{E}_5$ with $\mathcal{E}_8$	$\mathcal{E}_{10}$ with $\mathcal{E}_9$	$\mathcal{E}_{13}$ with $\mathcal{E}_{14}$
$\mathcal{E}_4$ with $\mathcal{E}_3$	$\mathcal{E}_7$ with $\mathcal{E}_8$	$\mathcal{E}_{12}$ with $\mathcal{E}_9$	$\mathcal{E}_{15}$ with $\mathcal{E}_{14}$

This computation yields a Final Element Ratio of ≈ 2.6

Examples

Example 2

We solve

$$\begin{cases} -\nabla \cdot \big((1.1 + \sin(\pi x)\sin(\pi y))\nabla u(x,y)\big) \\ \qquad\qquad = -3\cos^2(\pi x) + 4\cos^2(\pi x)\cos^2(\pi x) \\ \qquad\qquad\qquad +2.2\sin(\pi x)\sin(\pi y) + 2 - 3\cos^2(\pi y), & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega, \end{cases}$$

where $\Omega = [0,2] \times [0,2]$.

The exact solution is $u(x,y) = \sin(\pi x)\sin(\pi y)$.

Examples

We compute the average error using $\psi_1 \equiv 1/4$ and four point values using $\psi_2 \approx \delta_{(.5,.5)}$, $\psi_3 \approx \delta_{(.5,1.5)}$, $\psi_4 \approx \delta_{(1.5,1.5)}$, and $\psi_5 \approx \delta_{(1.5,.5)}$.

We use

$$\hat{\delta}_{(c_x,c_y)} = \frac{400}{\pi} e^{-400((x-c_x)^2+(y-c_y)^2)}$$

to approximate the delta function $\delta_{(c_x,c_y)}$.

Examples

Global Computation: We use a tolerance of 2% starting with an 8×8 mesh.

		ψ_1			ψ_2		
Lev.	Elt's	Est.	Err.	Rat.	Est.	Err.	Rat.
1	64	.035	.035	1.0	.090	.29	3.3
2	201	.0088	.0089	1.0	.042	.082	1.9
3	763	.0027	.0027	1.0	.020	.020	.99
4	2917	.00044	.00044	1.0	.0050	.00504	1.0

Examples

Global Computation: We use a tolerance of 2% starting with an 8×8 mesh.

		ψ_3		
Lev.	Elt's	Est.	Err.	Rat.
1	64	$.24$	$.022$	$.091$
2	201	$.0024$	$.014$	6.0
3	763	$.0020$	$.0020$	1.0
4	2917	$.0049$	$.00504$	1.0

Examples

Initial and final meshes. Final mesh has 2917 elements.

Examples

Decomposed Computation: Use data $\{\psi_1, \cdots, \psi_5\}$ independently using tolerances of 2%.

We vary the initial meshes; using 7×7 for $\hat{U}_1$; 9×9 for $\hat{U}_2$ and $\hat{U}_4$; and 12×12 for $\hat{U}_3$ and $\hat{U}_5$.

Data	Level	Elements	Estimate
ψ_1	3	409	$-.0004699$
ψ_2	4	1037	$-.007870$
ψ_3	2	281	$-.005571$
ψ_4	4	1037	$-.007870$
ψ_5	2	281	$-.005571$

The Final Element Ratio is ≈ 2.8.

Examples

Final meshes for $\{\hat{U}_1, \hat{U}_2, \hat{U}_3\}$.

Examples

Example 3

We solve

$$\begin{cases} -\Delta u = 16(y - y^2 + x - x^2) & (x, y) \in \Omega, \\ u(x, y) = 0, & (x, y) \in \partial\Omega, \end{cases}$$

where $\Omega = [0, 1] \times [0, 1]$.

The exact solution is $u(x, y) = 8x(1 - x)y(1 - y)$.

Examples

We estimate the error in the average value of u.

Since the domain is small and the solution and the generalized Green's function are very smooth, the gain from decomposing the solution is greatly reduced.

Beginning with a 4×4 mesh and using a tolerance of 1%, we obtain a sufficiently accurate solution using a Global Computation after five refinements.

The final mesh uses 885 elements and produces an error of $.0008699$.

Examples

If we partition the domain using four equal regions there are no substantial correlations.

Computing the four solutions independently in the Decomposed Computation yields a Final Element Ratio of around 1.5.

Examples

If we use sixteen equal regions, there are a number of substantial correlations.

Correlation Ratio 1 for $\mathcal{E}_1$ on $\mathcal{E}_2 = .98$,
Correlation Ratio 2 for $\mathcal{E}_1$ on $\mathcal{E}_2 = .44$,
Correlation Ratio 1 for $\mathcal{E}_2$ on $\mathcal{E}_1 = .82$,
Correlation Ratio 2 for $\mathcal{E}_2$ on $\mathcal{E}_1 = .44$.

Examples

Computing $\hat{U}_1$ corresponding to the localized data ψ_1 using a tolerance of 1% requires 367 elements.

Computing $\hat{U}_2$ requires a mesh 494 elements.

Combining these two computations by using data equal to the sum of the two partition functions for the regions Ω_1 and Ω_2 requires 496 elements.

We gain almost nothing by computing $\hat{U}_1$ and $\hat{U}_2$ independently

Examples

Final meshes.

Examples

We consider the error in the average value and the point values at $(.25, .25)$ and $(.5, .5)$.

We use a partition of unity decomposition for the error in the average to get data $\{\psi_1, \cdots, \psi_4\}$. We let $\psi_5 \approx \delta_{(.25,.25)}$ and $\psi_6 \approx \delta_{(.5,.5)}$.

We compare the correlation indicators on initial meshes ranging from 16 to 144 or 400 uniformly sized elements.

Examples

Correlation Ratios versus number of elements.

Examples

Correlation Ratios versus number of elements.

Examples

Correlation Ratios versus number of elements.

Examples

In general, we find that all Correlation Ratios converge to a limit as the number of elements increases.

Generally, the second Correlation Ratio varies relatively little as the mesh density increases for all data.

The first Correlation Ratio between data representing a partition of unity decomposition also varies relatively little.

The first Correlation Ratio varies quite a bit on coarse meshes when one of the data is an approximate delta function.

Examples

The determination that two effective domains of influence are **not** closely correlated is relatively robust with respect to the density of the mesh.

There is a mild tendency to combine computations that are more efficiently treated independently if the correlation indicators are computed on very coarse meshes.

Examples

Example 4

We solve

$$\begin{cases} -\nabla \cdot \Big(\big(.05 + \tanh\big(10(x-5)^2 + 10(y-1)^2\big)\big) \nabla u \Big) \\ \qquad\qquad\qquad\qquad\qquad\qquad + \begin{pmatrix} -100 \\ 0 \end{pmatrix} \cdot \nabla u = 1, & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega, \end{cases}$$

where $\Omega = [0,10] \times [0,2]$.

Examples

Plot of the diffusion coefficient.

Examples

We use an initial mesh of 80 elements and an error tolerance of $TOL = .04\%$.

Level	Elements	Estimate
1	80	$-.0005919$
2	193	$-.001595$
3	394	$-.0009039$
4	828	$-.0003820$
5	1809	$-.0001070$
6	3849	$-.00004073$
7	9380	$-.00001715$
8	23989	$-.000007553$

Examples

Final Mesh.

Examples

Pe=1000

Pe=.1

Plots of the meshes for the original problem with $Pe = 1000$ and a problem with $Pe = .1$.

Examples

11	12	13	14	15	16	17	18	19	20
1	2	3	4	5	6	7	8	9	10

Domains for the partition of unity.

Examples

Significant Correlations:

$\mathcal{E}_3$ with $\mathcal{E}_4$	$\mathcal{E}_6$ with $\mathcal{E}_7$	$\mathcal{E}_7$ with $\mathcal{E}_6$	$\mathcal{E}_9$ with $\mathcal{E}_8$	$\mathcal{E}_{10}$ with $\mathcal{E}_8$, $\mathcal{E}_9$
$\mathcal{E}_{13}$ with $\mathcal{E}_{14}$	$\mathcal{E}_{16}$ with $\mathcal{E}_{17}$	$\mathcal{E}_{17}$ with $\mathcal{E}_{16}$	$\mathcal{E}_{19}$ with $\mathcal{E}_{18}$	$\mathcal{E}_{20}$ with $\mathcal{E}_{18}$, $\mathcal{E}_{19}$

Note, there are no significant correlations in the “cross-wind” direction.

Examples

Solutions are symmetric across $y = 1$.

Data	TOL	Level	Elements	Estimate
ψ_1	$.04\%$	7	7334	-6.927×10^{-7}
ψ_2	$.04\%$	7	8409	-5.986×10^{-7}
ψ_3	$.04\%$	7	7839	-5.189×10^{-7}
ψ_4	$.04\%$	7	7177	-5.306×10^{-7}
ψ_5	$.04\%$	7	7301	-4.008×10^{-7}
ψ_6	$.02\%$	7	6613	-2.471×10^{-7}
ψ_7	$.02\%$	7	4396	-2.938×10^{-7}
ψ_8	$.02\%$	7	4248	-1.656×10^{-7}
ψ_9	$.02\%$	7	3506	-1.221×10^{-7}
ψ_{10}	$.02\%$	7	1963	-5.550×10^{-8}

The Final Element Ratio is ≈ 2.9.

Examples

Final Mesh for $\hat{U}_1$

Final Mesh for $\hat{U}_5$

Plots of the final meshes for the localized solutions $\hat{U}_1$ and $\hat{U}_5$.

Examples

Final Mesh for $\hat{U}_9$

Plots of the final mesh for the localized solution $\hat{U}_9$.

Examples

Plots of the generalized Green's functions corresponding to ψ_{11} (left) and ψ_{19} (right).

Examples

The effective domains of influence may not be spatially compactly-shaped.

Examples

We combine some of the localized computations by solving for localized solutions corresponding to summing the two of the partition of unity data.

Data	TOL	Level	Elements	Estimate
$\psi_3 + \psi_4$	$.04\%$	7	8330	-9.8884×10^{-7}
$\psi_6 + \psi_7$	$.02\%$	7	5951	-5.897×10^{-7}
$\psi_8 + \psi_9$	$.02\%$	7	4406	-3.486×10^{-7}
$\psi_9 + \psi_{10}$	$.02\%$	7	3202	-2.243×10^{-7}

The solutions for $\psi_3 + \psi_4$ and $\psi_8 + \psi_9$ use a few more elements than required for either of the original localized solutions.

The solutions for $\psi_6 + \psi_7$ and $\psi_9 + \psi_{10}$ use less than the maximum required for the individual localized solutions.

Examples

Example 5

We solve

$$\begin{cases} -\frac{1}{\pi^2}\Delta u = 2 + 4e^{-5((x-.5)^2+(y-2.5)^2)}, & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega, \end{cases}$$

where Ω is the "square annulus" $\Omega = [0,3] \times [0,3] \setminus [1,2] \times [1,2]$.

The initial mesh has 48 elements and the error tolerance is 1%.

Examples

Level	Elements	Estimate
1	48	-5.168
2	125	-1.584
3	380	$-.6879$
4	894	$-.3029$
5	2075	$-.1435$

Examples

Initial and Final Meshes.

Examples

Solution and Generalized Green's Function on the Final Mesh.

Examples

7	6	5
8		4
1	2	3

The partition of unity has 8 square subdomains.

Examples

There are no significant correlations.

Data	Level	Elements	Estimate
ψ_1	5	1082	$-.01935$
ψ_2	5	1101	$-.01399$
ψ_3	5	1144	$-.01540$
ψ_4	5	1107	$-.01360$

Examples

There are no significant correlations.

Data	Level	Elements	Estimate
ψ_5	5	1104	$-.01436$
ψ_6	5	1110	$-.01587$
ψ_7	5	1074	$-.02529$
ψ_8	5	1098	$-.01660$

Final Element Ratio ≈ 1.8.

Examples

Final meshes.

Examples

Final meshes.

Examples

Plots of some Generalized Green's Functions.

Nonlinear Problems

A nonlinear algebraic equation

The problem is to estimate the error $e = x - X$ of a numerical solution X of a system of nonlinear algebraic equations,

$$f(x) = b$$

where the data b, nonlinearity f, and the solution x all have the same dimension.

The residual error is

$$R = f(X) - b$$

which immediately gives

$$f(x) - f(X) = -R.$$

The error is related to the residual through a nonlinear equation.

A nonlinear algebraic equation

The mean value theorem for integrals:

$$f(x) - f(X) = \int_0^1 f'(sx + (1-s)X)\,(x - X)\,ds$$

where f' is the Jacobian matrix of f.

We get

$$\tilde{A}e = -R$$

with

$$\tilde{A} = \int_0^1 f'(sx + (1-s)X)\,ds.$$

This is the linear problem obtained by linearizing f around an average of x and $-X$.

A nonlinear algebraic equation

We obtain

$$|(e,\psi)| = |(e,\tilde{A}^\top\phi)| = |(\tilde{A}e,\phi)| = |(R,\phi)|.$$

To obtain a computable adjoint problem, we can try to replace x by X in the definition of $\tilde{A}$,

$$\tilde{A} \to A = \int_0^1 f'(sX + (1-s)X)\,ds = f'(X),$$

But, what is the effect on the estimate?

Defining the adjoint to a nonlinear operator

We assume that the Banach spaces X and Y are Sobolev spaces and use $(\ ,\ )$ for the L^2 inner product, and so forth.

We define the adjoint for a specific kind of nonlinear operator.

We assume f is a nonlinear map from X into Y, where the domain $\mathcal{D}(f)$ is a convex set.

Definition
A subset A of a vector space is **convex** if for any $a, b \in A$, the set of points on the "line segment" joining a and b, i.e., $\{sa + (1-s)b |\, 0 \le s \le 1\}$ is contained in A.

Defining the adjoint to a nonlinear operator

We choose u inside $\mathcal{D}(f)$ and define

$$F(e) = f(u+e) - f(u),$$

where we think of e as representing an "error", i.e., $e = U - u$.

The domain of F is

$$\mathcal{D}(F) = \{v \in X \,|\, v + u \in \mathcal{D}(f)\}.$$

We assume that $\mathcal{D}(F)$ is independent of e and dense in X.

Note that $0 \in \mathcal{D}(F)$ and $F(0) = 0$.

We also assume that $\mathcal{D}(F)$ is a vector subspace of X.

Defining the adjoint to a nonlinear operator

Two reasons to work with functions of this form:

- This is the kind of nonlinearity that arises when estimating the error of a numerical solution or studying the effects of perturbations.
- Nonlinear problems typically do not enjoy the global solvability that characterizes linear problems, only a local solvability.

Defining the adjoint to a nonlinear operator

The first definition is based on the bilinear identity.

Definition
An operator $A^*(e)$ with domain $\mathcal{D}(A^*) \subset Y^*$ and range in X^* is an **adjoint operator** corresponding to F if

$$(F(e), w) = (e, A^*(e)w) \qquad \text{for all } e \in \mathcal{D}(F),\ w \in \mathcal{D}(A^*).$$

This is an adjoint operator associated with F, not the adjoint operator to F.

Defining the adjoint to a nonlinear operator

Example

Suppose that F can be represented as $F(e) = A(e)e$, where $A(e)$ is a linear operator with $\mathcal{D}(F) \subset \mathcal{D}(A)$.

For a fixed $e \in \mathcal{D}(F)$, define the adjoint of A satisfying

$$(A(e)w, v) = (w, A^*(e)v) \text{ for all } w \in \mathcal{D}(A),\ v \in \mathcal{D}(A^*).$$

Substituting $w = e$ shows this defines an adjoint of F as well.

If there are several such linear operators A, then there will be several different possible adjoints.

Defining the adjoint to a nonlinear operator

Example

Let $(t, x) \in \Omega = (0, 1) \times (0, 1)$, with $X = X^* = Y = Y^* = L^2$ denoting the space of periodic functions in t and x, with period equal to 1.

Consider a periodic problem

$$F(e) = \frac{\partial e}{\partial t} + e\frac{\partial e}{\partial x} + ae = f$$

where $a > 0$ is a constant and the domain of F is the set of continuously differentiable functions.

Defining the adjoint to a nonlinear operator

We can write $F(e) = A_i(e)e$ where

$$A_1(e)v = \frac{\partial v}{\partial t} + e\frac{\partial v}{\partial x} + av$$

$$A_2(e)v = \frac{\partial v}{\partial t} + \left(a + \frac{\partial e}{\partial x}\right) v$$

$$A_3(e)v = \frac{\partial v}{\partial t} + \frac{1}{2}\frac{\partial (ev)}{\partial x} + av.$$

Defining the adjoint to a nonlinear operator

The adjoints are

$$A_1^*(e)w = -\frac{\partial w}{\partial t} - \frac{\partial (ew)}{\partial x} + aw$$

$$A_2^*(e)w = -\frac{\partial w}{\partial t} + \left(a + \frac{\partial e}{\partial x}\right) w$$

$$A_3^*(e)w = -\frac{\partial w}{\partial t} - \frac{e}{2}\frac{\partial w}{\partial x} + aw.$$

Defining the adjoint to a nonlinear operator

We base the second definition of an adjoint on the integral mean value theorem.

We assume that the original nonlinearity is Frechet differentiable.

The integral mean value theorem states

$$f(U) = f(u) + \int_0^1 f'(u + se)\, ds\; e$$

where $e = U - u$ and f' is the Frechet derivative of f.

Defining the adjoint to a nonlinear operator

We rewrite this as

$$F(e) = f(U) - f(u) = A(e)e$$

with

$$A(e) = \int_0^1 f'(u + se)\, ds.$$

Note that we can apply the integral mean value theorem to F:

$$A(e) = \int_0^1 F'(se)\, ds.$$

To be precise, we should discuss the smoothness of F.

Defining the adjoint to a nonlinear operator

Definition

For a fixed e, the adjoint operator $A^*(e)$, defined in the usual way for the linear operator $A(e)$, is said to be an **adjoint** for F.

Example

Continuing the previous example,

$$F'(e)v = \frac{\partial v}{\partial t} + e\frac{\partial v}{\partial x} + \left(a + \frac{\partial e}{\partial x}\right) v.$$

After some technical analysis of the domains of the operators involved,

$$A^*(e)w = -\frac{\partial w}{\partial t} - \frac{e}{2}\frac{\partial w}{\partial x} + aw.$$

This coincides with the third adjoint computed above.

Analysis of a space-time finite element method

We study a system of D reaction-diffusion equations consisting of d parabolic equations and $D-d$ ordinary equations for the $\mathbb{R}^D$ valued function $u=(u_i)$:

$$\begin{cases} \dot{u}_i - \nabla\cdot(\epsilon_i(u,x,t)\nabla u_i) = f_i(u,x,t), & (x,t)\in\Omega\times\mathbb{R}^+,\ 1\le i\le D,\\ u_i(x,t)=0, & (x,t)\in\partial\Omega\times\mathbb{R}^+,\ 1\le i\le d,\\ u(x,0)=u_0(x), & x\in\Omega, \end{cases}$$

where there is a constant $\epsilon>0$ such that

$\epsilon_i(u,x,t)\ge\epsilon$ for $1\le i\le d$ and $\epsilon_i(u,x,t)\equiv 0$ for the rest.

Analysis of a space-time finite element method

Assumptions:

- Ω is a convex polygonal domain in $\mathbb{R}^2$ with boundary $\partial\Omega$
- $\epsilon = (\epsilon_i)$ and $f = (f_i)$ have smooth second derivatives

$\dot{u}_i$ denotes the time derivative of u_i

We write $\epsilon_i(u, x, t) = \epsilon_i(u)$ and $f(u, x, t) = f(u)$.

Analysis of a space-time finite element method

We use u^p and u^o to denote the parts of u associated to the parabolic and ordinary differential equations respectively.

$u_i^p = u_i$ for $1 \leq i \leq d$ and $u_i^p = 0$ for $d < i \leq D$

$u^o = u - u^p$

The presence of ordinary differential equations in the system has strong consequences for the smoothness of solutions.

Analysis of a space-time finite element method

Discretization of the space-time domain:

We partition $[0, \infty)$ as $0 = t_0 < t_1 < t_2 < \cdots < t_n < \ldots$, denoting each time interval by $I_n = (t_{n-1}, t_n]$ and time step by $k_n = t_n - t_{n-1}$.

To each interval I_n, we associate a triangulation $\mathcal{T}_n$ of Ω arranged so the union of the elements in $\mathcal{T}_n$ is Ω.

Analysis of a space-time finite element method

A space-time discretization.

Analysis of a space-time finite element method

As usual, we assume the intersection of any two elements in a space triangulation is either a common edge, node, or is empty.

We also assume that the smallest angle of any triangle in a triangulation is bounded below by a fixed constant

h_n denotes the piecewise constant mesh function $h_n|_K =$ diam(K) for $K \in \mathcal{T}_n$ and h denotes the global mesh function, where $h|_{I_n} = h_n$.

k denotes the piecewise constant function that is k_n on I_n.

Analysis of a space-time finite element method

The approximations are polynomials in time and piecewise polynomials in space on each space-time "slab" $S_n = \Omega \times I_n$.

$V_n \subset (H_0^1(\Omega))^d \times (H^1(\Omega))^{D-d}$ denotes the space of piecewise linear continuous vector-valued functions $v(x) \in \mathbb{R}^D$ defined on $\mathcal{T}_n$, where the first d components of v are zero on $\partial\Omega$.

We define

$$W_n^q = \left\{ w(x,t) : \, w(x,t) = \sum_{j=0}^{q} t^j v_j(x), \, v_j \in V_n, \, (x,t) \in S_n \right\}.$$

W^q denotes the space of functions defined on the space-time domain $\Omega \times \mathbb{R}^+$ such that $v|_{S_n} \in W_n^q$ for $n \geq 1$.

Analysis of a space-time finite element method

Functions in W^q are generally discontinuous across the discrete time levels.

$[w]_n = w_n^+ - w_n^-$, where $w_n^\pm = \lim_{s \to t_n \pm} w(s)$, denotes the jump across t_n

P_n is the L^2 projection onto V_n, i.e., $P_n : L^2(\Omega) \to V_n$ is defined by $(P_n v, w) = (v, w)$ for all $w \in V_n$. P is defined by $P = P_n$ on S_n.

$\pi_n : L^2(I_n) \to \mathcal{P}^q(I_n)$ denotes the L^2 projection onto the piecewise polynomial functions in time, where $\mathcal{P}^q(I_n)$ is the space of polynomials of degree q or less on I_n. π is defined by $\pi = \pi_n$ on S_n.

Analysis of a space-time finite element method

Definition
The **continuous Galerkin cG(q) approximation** $U \in W^q$ satisfies $U_0^- = P_0 u_0$ and for $n \geq 1$, the **Galerkin orthogonality relation**

$$\begin{cases} \displaystyle\int_{t_{n-1}}^{t_n} \big((\dot{U}_i, v_i) + (\epsilon_i(U)\nabla U_i, \nabla v_i)\big)\, dt = \int_{t_{n-1}}^{t_n} (f_i(U), v_i)\, dt \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for all } v \in W_n^{q-1},\ 1 \leq i \leq D, \\ U_{n-1}^+ = P_n U_{n-1}^-. \end{cases}$$

U is continuous across time nodes over which there is no mesh change.

Analysis of a space-time finite element method

Definition
The **discontinuous Galerkin dG(q) approximation** $U \in W^q$ satisfies $U_0^- = P_0 u_0$ and for $n \geq 1$,

$$\int_{t_{n-1}}^{t_n} \left((\dot{U}_i, v_i) + (\epsilon_i(U) \nabla U_i, \nabla v_i) \right) dt + \left([U_i]_{n-1}, v_i^+ \right)$$

$$= \int_{t_{n-1}}^{t_n} (f_i(U), v_i) \, dt$$

for all $v \in W_n^q$, $1 \leq i \leq D$.

Analysis of a space-time finite element method

Example

We discretize the scalar problem

$$\begin{cases} \dot{u} - \Delta u = f(u), & (x,t) \in \Omega \times \mathbb{R}^+, \\ u(x,t) = 0, & (x,t) \in \partial\Omega \times \mathbb{R}^+, \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases}$$

using the dG(0) method.

We let $\vec{U}_n$ denote the M_n vector of nodal values with respect to the nodal basis $\{\eta_{n,i}\}_{i=1}^{M_n}$ for V_n on I_n.

Analysis of a space-time finite element method

$B_n : \left(B_n\right)_{ij} = \left(\eta_{n,i}, \eta_{n,j}\right)$ for $1 \le i, j \le M_n$ and
$B_{n,n-1} : \left(B_{n,n-1}\right)_{ij} = \left(\eta_{n,i}, \eta_{n-1,j}\right)$ for $1 \le i \le M_n$,
$1 \le j \le M_{n-1}$ denotes the mass matrices

$A_n : \left(A_n\right)_{ij} = \left(\nabla\eta_{n,i}, \nabla\eta_{n,j}\right)$ denotes the stiffness matrices.

U_n satisfies

$$\left(B_n + k_n A_n\right)\vec{U}_n - \vec{F}(U_n^-)k_n = B_{n,n-1}\vec{U}_{n-1}, \quad n \ge 1,$$

where $(\vec{F}(U_n^-))_i = (f(U_n^-), \eta_{n,i})$.

Analysis of a space-time finite element method

Use of quadrature yields standard difference schemes

Example
If M_n is constant and the lumped mass quadrature is used to evaluate the coefficients of B_n and $B_{n,n-1} = B_n$, then the resulting set of equations for the dG(0) approximation is the same as the equations for the nodal values of the backward Euler difference scheme.

The dG(0) method is related to the backward Euler method, the cG(1) method is related to the Crank-Nicolson scheme, and the dG(1) method is related to the third order sub-diagonal Padé difference scheme.

Analysis of a space-time finite element method

Under general assumptions, the cG(q) and dG(q) have order of accuracy $q+1$ in time and 2 in space at any point.

In addition, they enjoy a superconvergence property in time at time nodes. The dG(q) method will have order of accuracy $2q+1$ in time and the cG(q) method will have order $2q$ in time at time nodes for sufficiently smooth solutions.

The discontinuous Galerkin method has stability properties that make it well suited for the solution of dissipative problems.

The continuous Galerkin method is “energy” preserving and is well-suited for problems with a conserved quantity.

Analysis of a space-time finite element method

We use the second definition of the adjoint, so use

$$\bar{\epsilon}_i = \bar{\epsilon}_i(u, U) = \int_0^1 \epsilon_i\big(us + U(1-s)\big)\, ds,$$

$$\bar{\beta}_{ij} = \bar{\beta}_{ij}(u, U) = \int_0^1 \frac{\partial \epsilon_j}{\partial u_i}\big(us + U(1-s)\big)\nabla\big(u_i s + U_i(1-s)\big)\, ds,$$

$$\bar{f}_{ij} = \bar{f}_{ij}(u, U) = \int_0^1 \frac{\partial f_j}{\partial u_i}\big(us + U(1-s)\big)\, ds.$$

Typically, $\bar{\epsilon}$ and $\bar{f}$ are piecewise continuous with respect to t and continuous, H^1 functions in space while $\bar{\beta}$ is discontinuous in time and space.

Analysis of a space-time finite element method

The adjoint problem is

$$\begin{cases} -\dot{\phi}_i - \nabla \cdot \left(\bar{\epsilon}_i \nabla \phi_i\right) + \sum_{j=1}^{D} \bar{\beta}_{ji} \cdot \nabla \phi_j - \sum_{j=1}^{D} \bar{f}_{ij} \phi_j = \psi_i, & \\ & (x,t) \in \Omega \times (t_n, 0],\ 1 \le i \le D, \\ \phi_i\left(x,t\right) = 0, & (x,t) \in \partial\Omega \times (t_n, 0], 1 \le i \le d, \\ \phi(x, t_n) = 0, & x \in \Omega, \end{cases}$$

Example

In the case of the scalar problem with constant diffusion, the adjoint problem is

$$\begin{cases} -\dot{\phi} - \epsilon \Delta \phi - \bar{f} \phi = \psi, & (x,t) \in \Omega \times (t_n, 0], \\ \phi(x,t) = 0, & (x,t) \in \partial\Omega \times (t_n, 0], \\ \phi(x, t_n) = 0, & x \in \Omega. \end{cases}$$

Analysis of a space-time finite element method

Example

In the case of one parabolic equation with nonlinear diffusion coupled to one ordinary differential equation, the dual problem is

$$\begin{cases} -\dot{\phi}_1 - \nabla \cdot \bar{\epsilon}_1 \nabla \phi_1 + \bar{\beta}_{11} \nabla \phi_1 - \bar{f}_{11} \phi_1 - \bar{f}_{12} \phi_2 = \psi_1, \\ -\dot{\phi}_2 + \bar{\beta}_{12} \nabla \phi_1 - \bar{f}_{21} \phi_1 - \bar{f}_{22} \phi_2 = \psi_2, \\ \phi_1(x,t) = 0, \\ \phi(x,t_n) = 0. \end{cases}$$

Analysis of a space-time finite element method

For the cG method, we obtain

$$\int_0^{t_n} (e, \psi)\, dt = (e^+(0), \phi(0))$$
$$+ \int_0^{t_n} \big((\dot{U}, \pi P\phi - \phi) + (\epsilon(U)\nabla U, \nabla(\pi P\phi - \phi)) - (f(U), \pi P\phi - \phi) \big)\, dt.$$

For the dG method, we obtain

$$\int_0^{t_n} (e, \psi)\, dt = (e^-(0), \phi(0)) + \sum_{j=1}^{n} \big([U]_{j-1}, (\pi P\phi - \phi)^+_{j-1} \big)$$
$$+ \int_0^{t_n} \big((\dot{U}, \pi P\phi - \phi) + (\epsilon(U)\nabla U, \nabla(\pi P\phi - \phi)) - (f(U), \pi P\phi - \phi) \big)\, dt.$$

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