Minitutorial on A Posteriori Error Estimation

Donald Estep

University Interdisciplinary Research Scholar
Editor in Chief, SIAM/ASA Journal on Uncertainty Quantification
SIAM Fellow
Chalmers Jubilee Professor
Department of Statistics
Colorado State University

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Collaborators and Colleagues

This minitutorial describes developments in a posteriori error analysis over a period of more than twenty years.

The approach is built on a foundation of functional analysis that has a broader application than just numerical analysis.

My own contributions result from collaborations with a number of senior people, students, and postdocs.

Significant contributions have been made by many other colleagues.

I give a few references at the end and these contain further references.
A Priori and A Posteriori Analysis

Two general approaches to analyzing numerical methods:

- **a priori** The goal is to derive the general convergence and accuracy properties of a numerical method for a wide class of solutions.
- **a posteriori** The goal is to derive a computational estimate that evaluates the accuracy of information computed from a particular numerical solution.

A priori analysis is the “classic” error analysis that dominates the research literature.

A priori analysis is generally useless for determining the accuracy of a particular computation.

A posteriori analysis techniques yield accurate error estimates but do not describe general approximation properties well.
Functionals, Dual Spaces, and Adjoint Tools for Investigating Differential Equations
We investigate properties of operators (maps) between spaces.

We often assume the spaces in question are Banach spaces.

A Banach space is a normed vector space such that Cauchy sequences converge to a limit in the space.

A sequence \( \{x_n\} \) in a space \( X \) is a Cauchy sequence if 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.
The starting point is the computation of particular information, or a quantity of interest, obtained from a numerical solution of a model.

Considering a particular quantity of interest is important because obtaining solutions that are accurate everywhere is often impossible.

The application should begin by answering

What do we want to compute from the model?
Definition of Linear Functionals

Let $X$ be a vector space with norm $\| \|$.

A bounded linear functional $\ell$ is a continuous linear map from $X$ to the reals $\mathbb{R}$, $\ell \in \mathcal{L}(X, \mathbb{R})$.

A linear functional is a one dimensional “snapshot” of a vector.

For $v$ in $\mathbb{R}^n$ fixed, the map

$$\ell(x) = v \cdot x = (x, v)$$

is a linear functional on $\mathbb{R}^n$.

The linear functional on $\mathbb{R}^n$ given by the inner product with the basis vector $e_i$ gives the $i^{th}$ component of a vector.
Definition of Linear Functionals

For a continuous function \( f \) on \([a, b]\),

\[
\ell(f) = \int_{a}^{b} f(x) \, dx \quad \text{and} \quad \ell(f) = f(y) \quad \text{for} \quad a \leq y \leq b
\]

are linear functionals.

Statistical moments like the expected value \( E(X) \) of a random variable \( X \) are linear functionals.

The Fourier coefficients of a continuous function \( f \) on \([0, 2\pi]\),

\[
c_j = \int_{0}^{2\pi} f(x) \, e^{-ijx} \, dx
\]

are linear functionals of \( f \).
Sets of Linear Functionals

Presumably, it is easier to compute accurate snapshots than the entire functions

We may use a set of snapshots to attempt to describe a function

In many situations, we settle for an “incomplete” set of snapshots

We are often happy with a small set of moments of a random variable

In practical applications of Fourier series, we truncate the infinite series to a finite number of terms,

\[ \sum_{j=-\infty}^{\infty} c_je^{ijx} \rightarrow \sum_{j=-J}^{J} c_je^{ijx} \]
Are There Many linear functionals?

Are there many bounded linear functionals on an arbitrary normed vector space?

The celebrated Hahn-Banach theorem provides a way to generate a large number of linear functionals.

**Hahn-Banach Theorem** 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

We are interested in the structure of the set of all linear functionals.

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

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

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

size = largest value of the snapshot on vectors of length 1.
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 bounded since

\[ |(x, v)| \leq \|v\| \|x\| = C\|x\| \]

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

\[ (\mathbb{R}^n)^* \simeq \mathbb{R}^n \]
Recall Hölder’s inequality: if \( f \in L^p(\Omega) \) and \( g \in L^q(\Omega) \) with 
\[
p^{-1} + q^{-1} = 1 \quad \text{for} \quad 1 \leq p, q \leq \infty ,
\]
then 
\[
\|fg\|_{L^1(\Omega)} \leq \|f\|_{L^p(\Omega)} \|g\|_{L^q(\Omega)}
\]

Each \( g \) in \( L^q(\Omega) \) is associated with a bounded linear functional on \( L^p(\Omega) \) when 
\[
p^{-1} + q^{-1} = 1 \quad \text{and} \quad 1 \leq p, q \leq \infty
\]
by
\[
F(f) = \int_{\Omega} g(x) f(x) \, dx
\]

We can “identify” \((L^p)^*\) with \( L^q \) for \( 1 < p, q < \infty, \ p^{-1} + q^{-1} = 1 \)

The cases \( p = 1, q = \infty \) and \( p = \infty, q = 1 \) are trickier
Hilbert spaces are Banach spaces with an inner product $(\ , \ )$

$\mathbb{R}^n$ and $L^2$ are Hilbert spaces

If $X$ is a Hilbert space, then $\psi \in X$ determines a bounded linear functional via the inner product

$$\ell_\psi(x) = (x, \psi), \quad x \in X$$

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

We can identify the dual space of a Hilbert space with itself

Linear functionals are commonly represented as inner products
Some useful choices of Riesz representors $\psi$ for functions $f$:

- $\psi = \chi_\omega/|\omega|$ gives the error in the average value of $f$ over a subset $\omega \subset \Omega$, where $\chi_\omega$ is the characteristic function of $\omega$.
- $\psi = \delta_c$ gives the average value $\oint_c f(s) \, ds$ of $f$ on a curve $c$ in $\mathbb{R}^n$, $n = 2, 3$, and $\psi = \delta_s$ gives the average value of $f$ over a plane surface $s$ in $\mathbb{R}^3$ ($\delta$ denotes the corresponding delta function).
- We can obtain average values of derivatives using dipoles similarly.
- $\psi = f/\|f\|$ gives the $L^2$ norm of $f$.

Only some of these $\psi$ have spatially local support.
We “borrow” the Hilbert space notation for the general case:

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

$$y(x) = \langle x, y \rangle$$

This is called the bracket notation

The generalized Cauchy inequality is

$$|\langle x, y \rangle| \leq \|x\|_X \|y\|_{X^*}, \quad x \in X, \ y \in X^*$$
Motivation for the Adjoint Operator

Let $X, Y$ be normed vector spaces

Assume that $L \in \mathcal{L}(X, Y)$ is a continuous linear map

The goal is to compute a snapshot or functional value of the output

$$\ell(L(x)), \text{ some } x \in X$$

Some important questions:

- Can we find a way to compute the snapshot value efficiently?
- What is the error in the snapshot value if approximations are involved?
- Given a collection of snapshot values, what can we say about $L$?
- Given a snapshot value, what can we say about $x$?
Definition of the Adjoint Operator

Let $X$, $Y$ be normed vector spaces with dual spaces $X^*$, $Y^*$

Assume that $L \in \mathcal{L}(X, Y)$ is a continuous linear map

For each $y^* \in Y^*$ there is an $x^* \in X^*$ defined by

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

snapshot of $x$ in $X$ = snapshot of image $L(x)$ of $x$ in $Y$

The adjoint map $L^* : Y^* \rightarrow X^*$ satisfies the bilinear identity

$$\langle L(x), y^* \rangle = \langle x, L^*(y^*) \rangle, \quad x \in X, \ y^* \in Y^*$$
Let $X = \mathbb{R}^m$ and $Y = \mathbb{R}^n$ with the standard inner product and norm

$L \in \mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)$ is associated with a $n \times m$ matrix $A$:

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

and

$$y_i = \sum_{j=1}^{m} a_{ij} x_j, \quad 1 \leq i \leq n$$
Adjoint of a Matrix

The bilinear identity reads

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

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

\[L^*y^*(x) = y^*(L(x)) = \begin{pmatrix} y_1^*, \ldots, y_n^* \end{pmatrix} \begin{pmatrix} \sum_{j=1}^m a_{1j}x_j \\ \vdots \\ \sum_{j=1}^m a_{nj}x_j \end{pmatrix} = \sum_{j=1}^m y_1^* a_{1j}x_j + \cdots + \sum_{j=1}^m y_n^* a_{nj}x_j = \sum_{j=1}^m \left( \sum_{i=1}^n y_i^* a_{ij} \right) x_j \]
Adjoint of a Matrix

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

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

The matrix $A^*$ of $L^*$ is

$$A^* = \begin{pmatrix} a_{11}^* & \cdots & a_{1n}^* \\ \vdots & \ddots & \vdots \\ a_{m1}^* & \cdots & a_{mn}^* \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ \vdots & \ddots & \vdots & \vdots \\ a_{1m} & a_{2m} & \cdots & a_{nm} \end{pmatrix} = A^\top.$$
We can define $L^*$ for a linear operator $L : X \to Y$ by considering $L$ on a dense subset of $X$.

We define the adjoint to the restriction of $L$ on a dense subset of $X$.

If this “restricted” adjoint is uniformly continuous on the dense subset, then the Hahn-Banach theorem implies that the restriction can be extended continuously to all of $X$.

This is useful in the weak formulation of differential equations in Sobolev spaces.
Theorem Let \( X, Y, \) and \( Z \) be normed linear spaces. For \( L_1, L_2 \in \mathcal{L}(X, Y) \):

\[
L_1^* \in \mathcal{L}(Y^*, X^*) \\
\|L_1^*\| = \|L_1\| \\
0^* = 0 \\
(L_1 + L_2)^* = L_1^* + L_2^* \\
(\alpha L_1)^* = \alpha L_1^*, \quad \text{all } \alpha \in \mathbb{R}
\]

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

\[
(L_1 L_2)^* = L_2^* L_1^*.
\]
The adjoint of the differential operator $L$

$$(Lu, v) \rightarrow (u, L^*v)$$

is obtained by a succession of integration by parts

Boundary terms involving functions and derivatives arise from each integration by parts

We use a two step process

1. We first compute the formal adjoint by assuming that all functions have compact support and ignoring boundary terms

2. We then compute the adjoint boundary and data conditions to make the bilinear identity hold
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 gives

\[- \int_{0}^{1} \frac{d}{dx} \left( a(x) \frac{d}{dx} u(x) \right) v(x) \, dx \]

\[ = \left[ a(x) \frac{d}{dx} u(x) \frac{d}{dx} v(x) \right]_{0}^{1} - \int_{0}^{1} a(x) \frac{d}{dx} u(x) \frac{d}{dx} v(x) \, dx \]

\[ = -\left[ u(x) \frac{d}{dx} \left( a(x) \frac{d}{dx} v(x) \right) \right]_{0}^{1} + u(x)a(x) \frac{d}{dx} v(x) \]
Formal Adjoints

\[ \int_0^1 \frac{d}{dx} (b(x)u(x))v(x) \, dx \]

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

Neglecting boundary terms gives the formal adjoint

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

\[ \implies L^*v = - \frac{d}{dx} \left( a(x) \frac{d}{dx} v(x) \right) - b(x) \frac{d}{dx} (v(x)) \]
In higher space dimensions, we use the divergence theorem

A general linear second order differential operator $L$ in $\mathbb{R}^n$:

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

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

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

It can be verified directly that

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

where

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

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 \( \partial \Omega \).
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

\[ va_{11} \frac{\partial^2 u}{\partial x_1^2} - u \frac{\partial^2 (a_{11} v)}{\partial x_1^2} = \frac{\partial}{\partial x_1} \left( a_{11} v \frac{\partial u}{\partial x_1} - u \frac{\partial (a_{11} v)}{\partial x_1} \right). \]
Important examples:

\[
\text{grad}^* = -\text{div} \\
\text{div}^* = -\text{grad} \\
\text{curl}^* = \text{curl}
\]

\[
L u = \sum_{|\alpha| \leq p} a_\alpha(x) D^\alpha u
\]

then

\[
L^* v = \sum_{|\alpha| \leq p} (-1)^{|\alpha|} D^\alpha (a_\alpha(x) v(x)).
\]
In the second stage, we deal with the boundary terms that arise during integration by parts.

The standard adjoint boundary conditions are the minimal conditions required so the bilinear identity holds true.

The form of the boundary conditions imposed on the differential operator is important, but not the values.

We assume homogeneous boundary values for the differential operator when determining the adjoint conditions.

We may need to use other boundary conditions, e.g. if the quantity of interest is determined on a boundary.
Consider
\[
\begin{cases}
  s''(x) = f(x), & 0 < x < 1, \\
  s(0) = s'(0) = 0
\end{cases}
\]

Integrating by parts,
\[
\int_0^1 (s''v - sv'') \, dx = (vs' - sv') \bigg|_0^1
\]

The boundary conditions imply the contributions at \( x = 0 \) vanish, while at \( x = 1 \) we have
\[
v(1)s'(1) - v'(1)s(1)
\]

The adjoint boundary conditions are \( v(1) = v'(1) = 0 \) since we cannot specify \( s'(1) \) or \( s(1) \)
Recall

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

The Dirichlet and Neumann boundary value problems for the Laplacian are their own adjoints.
Adjoint Boundary Conditions

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

$$\begin{cases} -\Delta v = g, & x \in \Omega, \\ \frac{\partial v}{\partial n} - \frac{\partial v}{\partial s} = 0, & x \in \partial \Omega. \end{cases}$$
For an initial value problem, we have $\frac{d}{dt}$ and an initial condition

Now

$$\int_0^T \frac{du}{dt} v \, dt = u(t)v(t) \bigg|_0^T - \int_0^T u \frac{dv}{dt} \, dt$$

The boundary term at 0 vanishes because $u(0) = 0$

The adjoint is a final-value problem with “initial” condition $v(T) = 0$

The adjoint problem has $-\frac{dv}{dt}$ and time “runs backwards”
Adjoint for an Evolution Operator

\[
\begin{aligned}
Lu = \frac{du}{dt} - \Delta u &= f, \quad x \in \Omega, \ 0 < t \leq T, \\
u = 0, \quad &x \in \partial\Omega, \ 0 < t \leq T, \\
u = u_0, \quad &x \in \Omega, \ t = 0
\end{aligned}
\]

\[
\begin{aligned}
L^*v = -\frac{dv}{dt} - \Delta v &= \psi, \quad x \in \Omega, \ T > t \geq 0, \\
v = 0, \quad &x \in \partial\Omega, \ T > t \geq 0, \\
v = 0, \quad &x \in \Omega, \ t = T
\end{aligned}
\]

A useful alternative is

\[
\begin{aligned}
L^*v = -\frac{dv}{dt} - \Delta v &= 0, \quad x \in \Omega, \ T > t \geq 0, \\
v = 0, \quad &x \in \partial\Omega, \ T > t \geq 0, \\
v = \psi, \quad &x \in \Omega, \ t = T
\end{aligned}
\]
The Usefulness of Duality and Adjoints
The dual space can be better behaved than the original normed vector space

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

This can be exploited in analysis in $X$, e.g. “weak” convergence results
There is an intimate connection between the adjoint operator and the stability properties of the original operator.

The singular values of a matrix $L$ are the square roots of the eigenvalues of the square, symmetric transformations $L^*L$ or $LL^*$.

This connects the condition number of a matrix $L$ to $L^*$.
Given normed vector spaces $X$ and $Y$, an operator $L(X, Y)$, and $b \in Y$, find $x \in X$ such that

$$Lx = b$$

A necessary condition that $b$ is in the range of $L$ is $y^*(b) = 0$ for all $y^*$ in the null space of $L^*$.

This is a sufficient condition if the range of $L$ is closed in $Y$.

If $A$ is an $n \times m$ matrix, a necessary and sufficient condition for the solvability of $Ax = b$ is $b$ is orthogonal to all linearly independent solutions of $A^T y = 0$. 

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When $X$ is a Hilbert space and $L \in \mathcal{L}(X, Y)$, then the range of $L^*$ is a subset of the orthogonal complement of the null space of $L$.

If the range of $L^*$ is “large”, then the orthogonal complement of the null space of $L$ must be “large” and the null space of $L$ must be “small”.

The existence of sufficiently many solutions of the homogeneous adjoint equation $L^* \phi = 0$ implies there is at most one solution of $Lu = b$ for a given $b$.

This is the basis for the Holmgren Uniqueness Theorem in PDEs.
Suppose we wish to compute a functional $\ell(x)$ of the solution $x \in \mathbb{R}^n$ of a $n \times n$ system

$$Lx = b$$

For a linear functional $\ell(\cdot) = (\cdot, \psi)$, we define the adjoint problem

$$L^* \phi = \psi$$

Variational analysis yields the representation formula

$$\ell(x) = (x, \psi) = (x, L^* \phi) = (Lx, \phi) = (b, \phi)$$

We can compute many solutions by computing one adjoint solution and taking inner products.
Green’s Functions

For

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

the Green’s function solves

\[ -\Delta \phi = \delta_x \quad (\text{delta function at } x) \]

This yields

\[ u(x) = (u, \delta_x) = (f, \phi) \]

The generalized Green’s function solves the adjoint problem with general functional data, rather than just \( \delta_x \)

The imposition of the adjoint boundary conditions is crucial
Nonlinear Operators

(13)
There is no unique “natural” adjoint for a general 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 of $f$ is a convex set
A Perturbation Operator

Consider a “true” \( u \) and “approximation” \( U \) in the domain of \( f \) and define the “error” \( e = U - u \)

\( u \) and \( e \) are “unknown”

Define

\[
F(e) = f(u + e) - f(u),
\]

The domain of \( F \) is

\[
\{ v \in X | v + u \in \text{domain of } f \}\]

Assume the domain of \( F \) is independent of \( e \) and dense in \( X \)

Note that 0 is in the domain of \( F \) and \( F(0) = 0 \)
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.
Definition 1

A common definition is based on the bilinear identity

An operator $A^*(e)$ is an adjoint operator corresponding to $F$ if

$$(F(e), w) = (e, A^*(e)w) \quad \text{for all } e \in \text{domain of } F, \ w \in \text{domain of } A^*$$

This is an adjoint operator associated with $F$, not the adjoint operator to $F$
Definition 1

Suppose that $F$ can be represented as $F(e) = A(e)e$, where $A(e)$ is a linear operator with the domain of $F$ contained in the domain of $A$

For a fixed $e$ in the domain of $F$, define the adjoint of $A$ satisfying

$$(A(e)w, v) = (w, A^*(e)v)$$

for all $w \in \text{domain of } A$, $v \in \text{domain of } A^*$

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

\[
A_1(e)v = \frac{\partial v}{\partial t} + e \frac{\partial v}{\partial x} + av \implies A_1^*(e)w = -\frac{\partial w}{\partial t} - \frac{\partial (ew)}{\partial x} + aw
\]

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

\[
A_3(e)v = \frac{\partial v}{\partial t} + \frac{1}{2} \frac{\partial (ev)}{\partial x} + av \implies A_3^*(e)w = -\frac{\partial w}{\partial t} - \frac{e}{2} \frac{\partial w}{\partial x} + aw
\]
If the nonlinearity is Frechet differentiable, we base the second definition of an adjoint on the integral mean value theorem.

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 \( f \).
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 \( F \)
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 $F$.

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.
A Point about Linearization

The linearization approach is used in many practical applications

Typically the linearization in the integral mean value theorem is approximated by linearization at a “known” point

This raises the issue of the effect of such linearization “error” on any subsequent use of the adjoint

For many analysis purposes, the issue is the accuracy of the inverse of the approximation
A Point about Linearization

Consider \( F : \mathbb{R}^2 \rightarrow \mathbb{R}^2 : \)

\[
F(u) = \begin{pmatrix}
u_1^2 + 3u_2 \\
u_1 e^{u_2}
\end{pmatrix}
\]

For perturbation \( \varepsilon = (\varepsilon_1, \varepsilon_2) \top \),

\[
\mathcal{E}(\varepsilon) = F(u + \varepsilon) - F(u) = \begin{pmatrix}
2u_1 + \varepsilon_1 \\
e^{u_2+\varepsilon_2} \\
u_1 e^{u_2} \left( \frac{e^{\varepsilon_2}-1}{\varepsilon_2} \right)
\end{pmatrix} \begin{pmatrix}
\varepsilon_1 \\
\varepsilon_2
\end{pmatrix}
\]

This yields

\[
\mathcal{E}(\varepsilon)^* = \begin{pmatrix}
2u_1 + \varepsilon_1 \\
3 \\
u_1 e^{u_2} \left( \frac{e^{\varepsilon_2}-1}{\varepsilon_2} \right)
\end{pmatrix}
\]
A Point about Linearization

For small $\varepsilon$,

$$\mathcal{E}(\varepsilon)^* \approx (F'(u))^*$$

where $F'(u)$ is the Jacobian,

$$F'(u) = \begin{pmatrix} 2u_1 & 3 \\ e^{u_2} & u_1 e^{u_2} \end{pmatrix}$$

In practical computations, we use $F'(u)^*$

For $|u_1|$ bounded away from $\sqrt{3/2}$, $(F'(u)^*)^{-1} \approx (\mathcal{E}(v)^*)^{-1}$ for all $\varepsilon$ with sufficiently small norm

If $|u_1| \approx \sqrt{3/2}$, $(F'(u)^*)^{-1}$ may not be close to $(\mathcal{E}(\varepsilon)^*)^{-1}$
A Posteriori Error Analysis
Problem: Estimate the error in a quantity of interest computed using a numerical solution of a differential equation

We assume that the quantity of information can be represented as a linear functional of the solution

We use the adjoint problem associated with the linear functional
What about Convergence Analysis?

Recall the standard *a priori* convergence result for an initial value problem

\[
\begin{aligned}
\dot{y} &= f(y), \quad 0 < t, \\
y(0) &= y_0
\end{aligned}
\]

Let \( Y \approx y \) be an approximation associated with time step \( \Delta t \)

A typical *a priori* (Gronwall argument) bound is

\[
\| Y - y \|_{L^\infty(0,t)} \leq C e^{Lt} \Delta t^p \left\| \frac{d^{p+1}y}{dt^{p+1}} \right\|_{L^\infty(0,t)}
\]

\( L \) is often large in practice, e.g. \( L \sim 100 - 10000 \)

It is typical for an *a priori* convergence bound to be orders of magnitude larger than the error
A Linear Algebra Problem

We compute a quantity of interest $(u, \psi)$ from a solution of

$$Au = b$$

If $U$ is an approximate solution, we estimate the error

$$(e, \psi) = (u - U, \psi)$$

We can compute the residual

$$R = AU - b$$

Using the adjoint problem $A^T\phi = \psi$, variational analysis gives

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

We solve for $\phi$ numerically to compute the estimate
Finite Element Method for Elliptic Problem

The a posteriori analysis naturally applies to finite element discretizations

Variational form of the equation is formed by multiplying by a test function, integrating over space and time, and using integration by parts to reduce derivative orders

Appropriate function spaces must be chosen

The finite element approximation uses finite dimensional function spaces, e.g. piecewise polynomials

Finite volume and finite difference methods are written as finite elements + quadrature
Approximate $u : \mathbb{R}^n \to \mathbb{R}$ solving

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

where

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

- $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$, is a convex polygonal domain
- $a = (a_{ij})$, where $a_{i,j}$ are continuous 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
- $c$ and $f$ are continuous
The variational formulation reads

Find $u \in H^1_0(\Omega)$ such that

$$A(u, v) = (a\nabla u, \nabla v) + (b \cdot \nabla u, v) + (cu, v) = (f, v)$$

for all $v \in H^1_0(\Omega)$

$H^1_0(\Omega)$ is the space of $L^2(\Omega)$ functions whose first derivatives are in $L^2(\Omega)$

This says that the solution solves the “average” form of the problem for a large number of weights $v$
We construct a triangulation of $\Omega$ into simplices, or elements, such that boundary nodes of the triangulation lie on $\partial \Omega$.

$\mathcal{T}_h$ denotes a simplex triangulation of $\Omega$ that is locally quasi-uniform, i.e. no arbitrarily long, skinny triangles.

We use the length of the longest edge $h_K$ of $K \in \mathcal{T}_h$ to quantify size.
Finite Element Method for Elliptic Problem

Triangulation of the domain $\Omega$

$U = 0$

$\mathcal{T}_h$

$h_K$

$K$

Triangulation of the domain $\Omega$
$V_h$ denotes the space of functions that are
- continuous on $\Omega$
- piecewise linear with respect to $\mathcal{T}_h$
- zero on the boundary

$V_h \subset H^1_0(\Omega)$, and for smooth functions, the error of interpolation into $V_h$ is $O(h^2)$ in $\|\|$.

The finite element method is:

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

This is Galerkin orthogonality since it is equivalent to

$A(U - u, v) = 0$ for all $v \in V_h$
We assume that quantity of interest is the functional \((u, \psi)\)

The generalized Green’s function \(\phi\) solves the weak adjoint problem: Find \(\phi \in H^1_0(\Omega)\) such that

\[
A^*(v, \phi) = (\nabla v, a \nabla \phi) - (v, \text{div} (b\phi)) + (v, c\phi) = (v, \psi)
\]

for all \(v \in H^1_0(\Omega),\)

corresponding to the adjoint problem \(L^*(D, x)\phi = \psi\)
A Posteriori Analysis for an Elliptic Problem

We now estimate the error $e = U - u$:

$$(e, \psi) = (\nabla e, a \nabla \phi) - (e, \text{div} (b \phi)) + (e, c \phi)$$

$$= (a \nabla e, \nabla \phi) + (b \cdot \nabla e, \phi) + (ce, \phi)$$

$$= (a \nabla u, \nabla \phi) + (b \cdot \nabla u, \phi) + (cu, \phi)$$

$$- (a \nabla U, \nabla \phi) - (b \cdot \nabla U, \phi) - (cU, \phi)$$

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

The weak residual of $U$ is

$$R(U, v) = (f, v) - (a \nabla U, \nabla v) - (b \cdot \nabla U, v) - (cU, v), \quad v \in H_0^1(\Omega)$$

$$R(U, v) = 0 \text{ for } v \in V_h \text{ but not for general } v \in H_0^1(\Omega)$$
A Posteriori Analysis for an Elliptic Problem

\( \pi_h \phi \) denotes an approximation of \( \phi \) in \( V_h \)

**Theorem** The error representation is,

\[
(e, \psi) = (f, \phi - \pi_h \phi) - (a \nabla U, \nabla (\phi - \pi_h \phi)) \\
- (b \cdot \nabla U, \phi - \pi_h \phi) - (c U, \phi - \pi_h \phi),
\]

Subtracting the projection \( \phi - \pi_h \phi \) is not needed theoretically but useful in practice

The subtraction is required for standard adaptive error control
A Posteriori Analysis for an Elliptic Problem

We approximate \( \phi \) using a higher order finite element method or on a significantly finer mesh.

For a second order elliptic problem, good results are obtained using the space \( V_h^2 \).

The approximate generalized Green's function \( \Phi \in V_h^2 \) solves

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

Theorem The approximate error representation is

\[
(e, \psi) \approx (f, \Phi - \pi_h \Phi) - (a\nabla U, \nabla (\Phi - \pi_h \Phi)) - (b \cdot \nabla U, \Phi - \pi_h \Phi) - (cU, \Phi - \pi_h \Phi)
\]
A Posteriori Analysis for an Elliptic Problem

\[
\begin{aligned}
-\Delta u &= 200\pi^2 \sin(10\pi x) \sin(10\pi y), & (x, y) &\in \Omega = [0, 1] \times [0, 1], \\
u &= 0, & (x, y) &\in \partial \Omega
\end{aligned}
\]

The solution is \( u = \sin(10\pi x) \sin(10\pi y) \)
We develop an estimate for

\[
\begin{aligned}
  \begin{cases}
    y' = f(y), & 0 < t \leq T, \\
    y(0) = y_0
  \end{cases}
\end{aligned}
\]

where \( f \) is smooth

Discretization of domain:

\[
0 = t_0 < t_1 < \cdots < t_N = T,
\]

\[
I_n = (t_{n-1}, t_n], \quad k_n = t_n - t_{n-1}, \quad k|_{I_n} = k_n
\]

Space of approximation:

\[
\mathcal{P}^q(I_n) = \text{polynomials of degree } q \text{ and less on } I_n
\]

\[
W^q_n = \{ w : w \in \mathcal{P}^q(I_n) \}, \quad W_n = \{ w : w|_{I_n} \in W^q_n \}
\]

\[
\pi_k = \text{interpolant/projection operator into } \mathcal{P}^q(I_n) \text{ for each } n
\]
The continuous Galerkin method of order $q$ (CG(q)): For $n = 1, \cdots, N$,

$$\begin{align*}
\left\{ \int_{I_n} (Y', v) \, dt & = \int_{I_n} (f(Y), v) \, dt \quad \text{all } v \in W_n^{q-1} \\
Y_{n-1}^+ & = Y_{n-1}^-
\right. \\
\text{with } Y_0 & = y_0, \quad U_n^+ = \lim_{t \downarrow t_n} U(t), \quad U_n^- = \lim_{t \uparrow t_n} U(t)
\end{align*}$$

There is a discontinuous Galerkin method

**Quantity of interest:** $\int_0^T (y, \psi) \, dt$

$\psi = 1/T$ gives the average value
Linearization to define adjoint:

\[ \bar{f}' = \overline{f'}(y, Y) = \int_0^1 \frac{\partial f}{\partial y}(sy + (1 - s)Y) \, ds \]

Adjoint problem:

\[
\begin{cases}
-\phi' = (\bar{f}')^* \phi, & T > t \geq 0, \\
\phi(T) = 0
\end{cases}
\]

time runs “backwards” but note the “-” on the time derivative

In practice, \( \bar{f}' \to f'(Y) \)
A Posteriori Analysis for an Initial Value Problem

Substituting

\[ \int_0^T (e, \psi) \, dt = \sum_{i=1}^N \int_{I_n} (e, -\phi' - (\bar{f}')^* \phi) \, dt \]

\[ \int_{I_n} (e, -\phi') \, dt = -(e_r^-, \phi_n) + (e_r^{+1}, \phi_n) + \int_{I_n} (e', \phi) \, dt \]

\[ \int_{I_n} (e, (\bar{f}')^* \phi) \, dt = \int_{I_n} (f(y) - f(Y), \phi) \, dt \]

**Theorem** The error representation is

\[ \int_0^T (e, \psi) \, dt = \sum_{n=1}^N \int_{I_n} (\mathcal{R}_n, \pi_k \phi - \phi) \, dt \]

\[ \mathcal{R}_n = Y' - f(Y) \text{ on } I_n \]
The chaotic Lorenz problem

\[
\begin{align*}
\dot{u}_1 &= -10u_1 + 10u_2, \\
\dot{u}_2 &= 28u_1 - u_2 - u_1u_3, \quad 0 < t, \\
\dot{u}_3 &= -\frac{8}{3}u_3 + u_1u_2,
\end{align*}
\]

Chaotic behavior affects numerical solutions as well
A Posteriori Analysis for an Initial Value Problem

2% error on [0,30]

100% error at t=18
The distance between the two numerical solutions
The errors follow an increasing trend, but decrease as well as increase
A Posteriori Analysis for an Initial Value Problem

The accuracy of the estimate in the pointwise error
A system of $D$ reaction-diffusion equations consisting of $d$ parabolic equations and $D - d$ ordinary equations for $u \in \mathbb{R}^D$:

$$
\begin{cases}
    u_i' - \nabla \cdot (\epsilon_i(u)\nabla u_i) = f_i(u), & (x, t) \in \Omega \times \mathbb{R}^+, \ 1 \leq i \leq D, \\
    u_i(x, t) = 0, & (x, t) \in \partial \Omega \times \mathbb{R}^+, \ 1 \leq i \leq d, \\
    u(x, 0) = u_0(x), & x \in \Omega,
\end{cases}
$$

Assumptions:

- $\epsilon_i(u) \geq \epsilon_0 > 0$ for $1 \leq i \leq d$ and $\epsilon_i(u) \equiv 0$ for the rest
- $\Omega$ is a convex polygonal domain with boundary $\partial \Omega$
- $\epsilon, f$ have smooth second derivatives
- $u_i^p = u_i$ for $1 \leq i \leq d$ and $u_i^p = 0$ for $d < i \leq D$
Discretization:

\[ 0 = t_0 < t_1 < t_2 < \cdots < t_N = T, \quad I_n = (t_{n-1}, t_n], \quad k_n = t_n - t_{n-1} \]

\( T_n \) is a triangulation of \( \Omega \) for \( t \in I_n \).
A Posteriori Analysis for a Reaction-Diffusion System

Discrete space: polynomials in time and piecewise polynomials in space on each space-time “slab” \( S_n = \Omega \times I_n \)

\[ V_n \subset (H^1_0(\Omega))^d \times (H^1(\Omega))^{D-d} \] denotes the space of piecewise linear continuous vector-valued functions \( v(x) \in \mathbb{R}^D \) defined on \( T_n \), where the first \( d \) components of \( v \) are zero on \( \partial \Omega \)

Define

\[ W^q_n = \{ w(x, t) : w(x, t) = \sum_{j=0}^{q} t^j v_j(x), v_j \in V_n, (x, t) \in S_n \}. \]

\( W^q \) denotes the space of functions defined on the space-time domain \( \Omega \times \mathbb{R}^+ \) such that \( v|_{S_n} \in W^q_n \) for \( n \geq 1 \)
The cG(q)-cG(1) approximation $U \in W^q$ satisfies $U_0^- = P_0 u_0$ and for $n \geq 1$,

$$\begin{cases}
\int_{t_{n-1}}^{t_n} ((U'_i, v_i) + (\epsilon_i(U) \nabla U_i, \nabla v_i)) \, dt = \int_{t_{n-1}}^{t_n} (f_i(U), v_i) \, dt \\
U_{n-1}^+ = P_n U_{n-1}^-
\end{cases}$$

for all $v \in W_{n-1}^{q-1}$, $1 \leq i \leq D$,

$P_n$ is the $L^2$ projection into $V_n$

The approximation is continuous across time nodes where there is no mesh change
A Posteriori Analysis for a Reaction-Diffusion System

Linearization for adjoint:

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

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

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

Adjoint problem:

\[
\begin{cases}
-\phi'_i - \nabla \cdot (\bar{\epsilon}_i \nabla \phi_i) + \sum_{j=1}^D \bar{\beta}_{ji} \cdot \nabla \phi_j - \sum_{j=1}^D \bar{f}_{ij} \phi_j = \psi_i, \\
\phi_i(x, t) = 0, \quad (x, t) \in \Omega \times (t_n, 0], \ 1 \leq i \leq D, \\
\phi_i(x, t_N) = 0, \quad x \in \Omega,
\end{cases}
\]
Theorem

\[
\int_0^T (e, \psi) \, dt = (u_0 - P_0 u_0, \phi(0)) \\
+ \sum_{n=1}^N \int_{I_n} (U', \pi_k \pi_h \phi - \pi_h \phi) + (\epsilon(U) \nabla U, \nabla (\pi_k \pi_h \phi - \pi_h \phi)) \\
- (f(U), \pi_k \pi_h \phi - \pi_h \phi) \, dt \\
+ \sum_{n=1}^N \int_{I_n} (U', \pi_h \phi - \phi) + (\epsilon(U) \nabla U, \nabla (\pi_h \phi - \phi)) \\
- (f(U), \pi_h \phi - \phi) \, dt
\]
Forward Error Propagation
Forward Error Propagation

We briefly describe the classic alternative for error estimation

For the initial value problem

\[ y' = f(y) \]

write the equation for a numerical solution \( Y \approx y \)

\[ Y' = F(Y) \]

where

\[ F(\cdot) \approx f(\cdot) \]
Subtraction yields an equation for the error \( e = y - Y \)

\[
e' = f(y) - F(Y) = f(y) - f(Y) + f(Y) - F(Y)
\]

Linearizing

\[
e' \approx f'(Y)e + \mathcal{R}(Y)
\]

with the defect \( \mathcal{R}(Y) = f(Y) - F(Y) \)

We can solve the system

\[
\begin{align*}
Y' &= F(Y), \\
e' &= f'(Y)e + \mathcal{R}(Y)
\end{align*}
\]

to compute the numerical solution and an approximation to the error simultaneously
Forward Error Propagation

Technical issues that must be addressed:

- The same issue regarding the choice of linearization point that affects the adjoint-based approach
- The defect must be interpreted in a correct mathematical sense
- The defect can be approximated in multiple ways without a clearly best choice

Computational evaluation of the two approaches:

- The forward propagation is cheaper when the goal is to estimate the error in the solution itself
- The adjoint-based method is cheaper when the goal is to estimate the error in a handful of quantity of interest functionals
My Preference

I prefer the adjoint-based approach because

▸ I have rarely encountered situations in which error in the solution is important

▸ The dual problem provides quantitative information about stability

▸ It seems easier to quantify relative contributions of different sources of error

▸ It seems easier to adapt the method to deal with such things as multiphysics, finite iteration, quadrature, etc.

A lot of nonsense is written about relative merits of the two approaches
Adjoint and Stability

(8)
The Adjoint and Stability

The solution of the adjoint problem scales local perturbations to global effects on a solution.

The adjoint problem carries stability information about the quantity of interest computed from the solution.

We can use the adjoint problem to investigate stability.
The classic error bound for an approximate solution $U$ of $Au = b$ is
\[ \|e\| \leq C\kappa(A)\|R\|, \quad R = AU - b \]

The **condition number** $\kappa(A) = \|A\| \|A^{-1}\|$ measures stability

\[ \kappa(A) = \frac{1}{\text{distance from } A \text{ to } \{\text{singular matrices}\}} \]

The **a posteriori** estimate $|(e, \psi)| = |(R, \phi)|$ yields
\[ |(e, \psi)| \leq \|\phi\| \|R\| \]

The **stability factor** $\|\phi\|$ is a weak condition number for the quantity of interest

We can obtain $\kappa$ from $\|\phi\|$ by taking the sup over all $\|\psi\| = 1$
We consider the problem of computing \((u, e_1)\) from the solution of

\[ Au = b \]

where \(A\) is a random \(800 \times 800\) matrix

The condition number is \(1.7 \times 10^5\)

The stability factor is \(16\)
The Condition of the Lorenz Problem
The Quantity of Interest is Important

The rate that errors grow depends strongly on the information being computed.

We consider the **average** distance from a solution to the origin over a long time interval.
The Quantity of Interest is Important

We compare to an ensemble average of 100 accurate solutions computed using time step .0001 for 15 time units.

<table>
<thead>
<tr>
<th>End Time</th>
<th>Coarse Solutions</th>
<th>Fine Solutions</th>
<th>Ensemble Ave</th>
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<td>Var</td>
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<tr>
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<td>26.3</td>
<td>83.7</td>
<td>26.3</td>
</tr>
</tbody>
</table>
The Bistable Problem

A parabolic problem:

\[
\begin{cases}
    u' - \epsilon \Delta u = u - u^3, & x \in \Omega, t > 0 \\
    \text{Neumann boundary conditions} & x \in \partial \Omega, t > 0 \\
    u(x, 0) = u_0(x), & x \in \Omega
\end{cases}
\]

Long time dynamics depends on space dimension

1D Metastable behavior of long periods of nearly motionless behavior punctuated by rapid transients

2D Approximate motion by mean curvature

The solutions in two dimensions are much more stable with respect to perturbations
The Bistable Problem

Example of metastable solution in one space dimension

Evolution of Solution

Norms of Adjoint Components
The Bistable Problem

Example of solution in two space dimensions

Evolution of Solution

Norms of Adjoint Solutions
Adjoint and Adaptive Error Control
The possibility of accurate error estimation suggests the possibility of optimizing discretizations.

Unfortunately, cancellation of errors significantly complicates the optimization problem.

In fact, there is no good theory for adaptive control of error.

There is good theory for adaptive control of error bounds.

The standard approach is based on optimal control theory.

The stability information in adjoint-based a posteriori error estimates is useful for this.
We consider the problem of computing \((u, e_1)\) from the solution of

\[
Au = b
\]

where \(A\) is a random \(800 \times 800\) matrix

The condition number of \(A\) is \(1.7 \times 10^5\)

estimate of the error in the quantity of interest \(\approx 1.4 \times 10^{-14}\)

\(a\) \textit{posteriori} error bound for the quantity of interest \(\approx 2.2 \times 10^{-10}\)

The traditional error bound for the error \(\approx 5.7 \times 10^{-5}\)
An abstract *a posteriori* error estimate has the form

\[ |(e, \psi)| = |(\text{Residual}, \text{Adjoint Weight})| \]

Given a tolerance TOL, a given discretization is refined if

\[ |(\text{Residual}, \text{Adjoint Weight})| \geq TOL \]

Refinement decisions are based on a bound consisting of a sum of element contributions

\[ |(e, \psi)| \leq \sum_{\text{elements } K} |(\text{Residual}, \text{Adjoint Weight})_K| \]

where \(( , )_K\) is the inner product on \(K\)

The element contributions in the bound do not cancel.
There is **no cancellation of errors across elements** in the bound, so optimization theory yields

**Principle of Equidistribution**: The optimal discretization is one in which the element contributions are equal

The **adaptive strategy** is to refine some of the elements with the largest element contributions

The adjoint weighted residual approach is different than traditional approaches because the element residuals are scaled by an adjoint weight, which measures how much error in that element affects the solution on other elements

An optimal solution is approximated iteratively starting with a coarse mesh
1: Choose error tolerance TOL and compute contribution tolerances
2: Choose initial coarse discretization parameters
3: Compute initial coarse solution
4: Compute error estimate for initial solution
5: while Error Estimate > TOL do
6: Adjust discretization parameters depending on the contributions relative to the contribution tolerances
7: Compute solution
8: Compute error estimate for solution
9: end while
\begin{align*}
\begin{cases}
-\nabla \cdot \left((.05 + \tanh(10(x - 5)^2 + 10(y - 1)^2))\nabla u\right) \\
+ \begin{pmatrix} -100 \\ 0 \end{pmatrix} \cdot \nabla u = 1, \quad (x, y) \in \Omega = [0, 10] \times [0, 2], \\
u = 0, \quad (x, y) \in \partial \Omega
\end{cases}
\end{align*}
Final meshes for an average error of 4% 24,000 elements versus 3500 elements
Treatment of Multiphysics Problems

(15)
Multiphysics, Multiscale Systems

Multiphysics, multiscale systems couple different physical processes interacting across a wide range of scales

Such systems abound in science and engineering application domains

Computational modeling plays a critical role in the predictive study of such systems

Some applications where multiphysics systems arise:

- Fusion and fission reactors
- Reacting fluids and fluid-solid interactions
- Advanced materials, nano-manufacturing
- Biological systems, drug design and delivery
- Environmental, climate, ecological models
- Weather models
Example: A MEMs Thermal Actuator

\[ \nabla \cdot (\sigma(d) \nabla V) = 0 \]
\[ \nabla \cdot (\kappa(T) \nabla T) = \sigma (\nabla V \cdot \nabla V) \]
\[ \hat{\nabla} \cdot (\lambda \text{tr}(E)I + 2\mu E - \beta (T - T_{ref})I) = 0 \]
\[ E = \left( \hat{\nabla} d + \hat{\nabla} d^\top \right) / 2 \]

electrostatic current
energy
displacement
Multiscale, multiphysics systems pose severe challenges for computational solution:

- Scale effects
- Complex stability
- Coupling between physics
- Different kinds of physical descriptions
- Mixtures of discretization methods and scales
- Complex HPC discretization techniques

Significant extensions of the a posteriori theory are required.
A simplified Thermal Actuator model:

\[
\begin{align*}
-\nabla \cdot a_1 \nabla u_1 + b_1 \cdot \nabla u_1 + c_1 u_1 &= f_1(x), \quad x \in \Omega, \\
-\nabla \cdot a_2 \nabla u_2 + b_2 \cdot \nabla u_2 + c_2 u_2 &= f_2(x, u_1, Du_1), \quad x \in \Omega, \\
u_1 = u_2 &= 0, \quad x \in \partial \Omega,
\end{align*}
\]

\(\Omega\) is a bounded domain with boundary \(\partial \Omega\)

The coefficients are smooth functions and \(a_1, a_2\) are bounded away from zero

We wish to compute information depending on \(u_2\)
Algorithm

- Construct discretizations $T_h,1$, $T_h,2$ and finite element spaces $V_{h,1}, V_{h,2}$
- Compute a finite element solution $U_1 \in V_{h,1}(\Omega)$ of the first equation
- Project $U_1 \in V_{h,1}(\Omega)$ into the space $V_{h,2}(\Omega)$
- Compute a finite element solution $U_2 \in V_{h,2}(\Omega)$ of the second equation

The projection between the discretization spaces is a crucial step

In a fully coupled system, $U_2$ is projected into $V_{h,1}(\Omega)$ for the next iteration
A Simple Thermal Actuator

Consider

\[ \begin{align*}
  -\Delta u_1 &= \sin(4\pi x) \sin(\pi y), & x \in \Omega \\
  -\Delta u_2 &= b \cdot \nabla u_1 = 0, & x \in \Omega, \\
  u_1 &= u_2 = 0, & x \in \partial \Omega,
\end{align*} \]

where \( \Omega = [0, 1] \times [0, 1] \)

We consider the quantity of interest

\[ u_2(.25, .25) \]

We solve for \( u_1 \) first and then solve for \( u_2 \) using independent meshes.
A Simple Thermal Actuator

Using uniform meshes, an a posteriori error estimate yields

\[
\text{estimate of the error in the quantity of interest} \approx 0.0042
\]

\[
\text{true error} \approx 0.0048
\]

\[
\text{discrepancy in estimate} \approx 0.0006 \ (\approx 13\%)
\]

This arises from the operator decomposition
A Simple Thermal Actuator

Adapting the mesh using only an error estimate for the second component causes the discrepancy to become alarmingly worse

estimate of the error in the quantity of interest $\approx 0.0001$

true error $\approx 0.2244$
We define **auxiliary quantities of interest** corresponding to information passed between components.

We solve auxiliary adjoint problems to estimate the error in that information.

In an iterative scheme, we also estimate the “history” of errors passed from one iteration level to the next.

We can also estimate the effect of processing, e.g. up and down scaling, the information.
Recall the “triangular” problem

\[
\begin{align*}
-\Delta u_1 &= \sin(4\pi x) \sin(\pi y), \quad x \in \Omega \\
-\Delta u_2 &= b \cdot \nabla u_1 = 0, \quad x \in \Omega, \\
u_1 &= u_2 = 0, \quad x \in \partial \Omega,
\end{align*}
\]

where \( \Omega = [0, 1] \times [0, 1] \)

We consider the quantity of interest

\[ u_2(.25, .25) \]

We solve for \( u_1 \) first and then solve for \( u_2 \) using independent meshes
\[
\begin{cases}
-\Delta u_1 = f_1(x), & x \in \Omega, \\
-\Delta u_2 = f_2(x, u_1, Du_1), & x \in \Omega \\
u_1 = 0, & x \in \partial \Omega
\end{cases}
\]

We compute a quantity of interest \((\psi^{(1)}, u)\) that only depends on \(u_2\), thus

\[
\psi^{(1)} = \begin{pmatrix} 0 \\ \psi_2^{(1)} \end{pmatrix}
\]

We require the linearization \(L f_2(w)\) of \(f_2\) with respect to \(u_1\) around the function \(w\)
The weak form of the primary adjoint problem is

\[
\begin{align*}
(\nabla \phi_1^{(1)}, \nabla v_1) + (Lf_2(U_1)\phi_2^{(1)}, v_1) &= 0, \\
(\nabla \phi_2^{(1)}, \nabla v_2) &= (\psi_2^{(1)}, v_2),
\end{align*}
\]

all test functions \(v_1, v_2\)

This yields the first error representation

\[
(\psi^{(1)}, e) = (f_2(u_1, Du_1), (I - \pi_h)\phi_2^{(1)}) - (\nabla U_2, \nabla (I - \pi_h)\phi_2^{(1)})
\]

The residual depends on the unknown true solution

We write

\[
f_2(u_1, Du_1) = f_2(U_2, DU_2) + (f_2(u_1, Du_1) - f_2(U_2, DU_2))
\]
We have a **new** linear functional of the error

\[
(f_2(u_1, Du_1) - f_2(U_1, DU_1), \phi_2^{(1)}) \approx (Lf(U_1)e_1, \phi_2^{(1)})
\]

\[
= (Lf(U_1)^* \phi_2^{(1)}, e_1) = (\psi^{(2)}, e)
\]

We pose a **secondary** adjoint problem

\[
\begin{cases}
(\nabla \phi_1^{(2)}, \nabla v_1) + (Lf_2(U_1) \phi_2^{(2)}, v_1) = (Lf_2(U_1)^* \phi_2^{(1)}, v_1) \\
(\nabla \phi_2^{(2)}, \nabla v_2) = 0
\end{cases}
\]

all test functions \( v_1, v_2 \)
Analysis for Multiscale, Multiphysics Solutions

Theorem

\[(\psi^{(1)}, e) = (f_2(U_1, DU_1), (I - \pi_h)\phi_2^{(1)}) - (\nabla U_2, \nabla (I - \pi_h)\phi_2^{(1)}) \]
\[+ (f_1, (I - \pi_h)\phi_1^{(2)}) - (\nabla U_1, \nabla (I - \pi_h)\phi_1^{(2)}) \]

\(\phi^{(1)}, \phi^{(2)}\) are the primary and secondary adjoint solutions

The new analysis estimates the error in the information passed between components

There is a tertiary adjoint problem and another term in the estimate if the different discretizations are used for the two components
If we adapt the meshes using all the terms in the estimate, we can drive the error below .0001.

We actually refine the mesh for $u_1$ more than the mesh for $u_2$. 
Extending to Other Discretizations

(16)
The a posteriori error analysis applies to wide classes of discretization.

The key is to write a chosen discretization method as some kind of finite element method with modifications such as quadrature to evaluate integrals.

Examples of extensions include:
- Finite difference schemes
- Finite volume methods
- Explicit and IMEX time integration methods
- Operator split discretizations

Extending the analysis always involves identifying new residuals and may involve defining additional adjoint problems.
Let $Q_r(g, n)$ denote a quadrature formula of order $r$ for the function $g$ on $I_n$

**CG(q) method with quadrature:** For $n = 1, \cdots, N$,

$$
\begin{cases}
\int_{I_n} (Y', v) \, dt = Q_r ((f(Y), n), v), n) \quad \text{all } v \in W_{nq}^{-1}
\end{cases}
$$

$$Y_{n-1}^+ = Y_{n-1}^-
$$

with $Y_0 = y_0$, $U_n^+ = \lim_{t \downarrow t_n} U(t)$, $U_n^- = \lim_{t \uparrow t_n} U(t)$

This yields a system of discrete equations determining $Y$

The discrete equations yield a finite difference scheme for $Y$
Consider $q = 1$ and the trapezoidal rule quadrature

On $I_n$,

$$Y = Y_n \frac{t - t_{n-1}}{k_n} + Y_{n-1} \frac{t_n - t}{k_n}$$

$$Q_1(g, n) = \frac{1}{2}(g(t_n) + g(t_{n-1}))k_n$$

The equation for the unknown coefficient $Y_n$ is

$$Y_n - \frac{1}{2} f(Y_n) k_n = Y_{n-1} + \frac{1}{2} f(Y_{n-1}) k_n$$
Key observation: Galerkin orthogonality uses $Q_r((f(Y), n), v), n)$ instead of exact integration.

We add and subtract $Q_r((f(Y), n), v), n)$ in the argument.

**Theorem** The error representation is

$$
\int_0^T (e, \psi) \, dt = \sum_{n=1}^N \int_{I_n} (R_n, \pi_k \phi - \phi) \, dt
$$

$$
+ \sum_{n=1}^N \left( \int_{I_n} (f(Y), \phi) \, dt - Q_r((f(Y), n), \phi), n) \right)
$$

$R_n = Y' - f(Y)$
Observations about the contribution to the error from quadrature

\[
\left( \int_{I_n} (f(Y), \phi) \, dt - Q_r((f(Y), n), \phi), n \right)
\]

- The stability factor is $\phi$ not $\pi_k \phi - \phi$, so this contribution accumulates at a different rate in general
- Exactly evaluating this expression requires exact integration of the nonlinear term, and this has to be approximated in general

Generically, such estimates include terms that cannot be evaluated exactly
Estimation of the effects of methods such as quadrature is important

We consider operator splitting for a reaction-diffusion problem

\[
\begin{aligned}
\frac{du}{dt} &= \Delta u + F(u), \quad 0 < t, \\
u(0) &= u_0
\end{aligned}
\]

The diffusion component \(\Delta u\) induces stability and change over long time scales

The reaction component \(F\) induces instability and change over short time scales
On \((t_{n-1}, t_n]\), we numerically solve
\[
\begin{aligned}
\frac{d u^R}{d t} &= F(u^R), \quad t_{n-1} < t \leq t_n, \\
u^R(t_{n-1}) &= u^D(t_{n-1})
\end{aligned}
\]

On \((t_{n-1}, t_n]\), we numerically solve
\[
\begin{aligned}
\frac{d u^D}{d t} - \Delta(u^D), \quad t_{n-1} < t \leq t_n, \\
u^D(t_{n-1}) &= u^R(t_n)
\end{aligned}
\]

The operator split approximation is \(u(t_n) \approx u^D(t_n)\)
Operator Splitting for Reaction-Diffusion Equations
We discretize using a finite element in time.

To account for the fast reaction, we approximate $u^r$ using many time steps inside each diffusion step.
Decompose the error using an exact operator split solution $u^s$:

$$u - U = (u - u^s) + (u^s - U)$$

- $u - u^s$: error of analytic operator splitting
  
  This is determined by properties of adjoint operators

- $u^s - U$: error of numerical component solves
  
  This is determined by the numerical errors made in each component

Estimates of the numerical error in each component do not indicate the effects of splitting in general
The Brusselator problem

\[
\begin{align*}
\frac{\partial u_i}{\partial t} - 0.025 \frac{\partial^2 u_i}{\partial x^2} &= f_i(u_1, u_2) \quad i = 1, 2 \\
f_1(u_1, u_2) &= 0.6 - 2u_1 + u_1^2 u_2 \\
f_2(u_1, u_2) &= 2u_1 - u_1^2 u_2
\end{align*}
\]

- Use a linear finite element method in space with 500 elements
- Use a standard first order splitting scheme
- Use Trapezoidal Rule with time step of \(0.2\) for the diffusion and Backward Euler with time step of \(0.004\) for the reaction
Instability in the Brusselator Operator Splitting

For large times, there is a critical step size above which there is no convergence. The instability is a direct consequence of the operator splitting.
Operator splitting complicates the definition of adjoint operators

- In a linear problem, the adjoint operators associated with the original problem and an operator split discretization are fundamentally different.

- Additionally in a nonlinear problem, the issue of choice of linearization point becomes complicated.

Estimates of the effects on adjoints cannot be entirely computable.
We derive a hybrid *a priori* - *a posteriori* estimate

\[(e(t_N), \psi) = Q_1 + Q_2 + Q_3\]

- **$Q_1$** estimates the contribution of the numerical solution of each component in a standard *a posteriori* way

- **$Q_2 \approx \sum_{n=1}^{N} (U_{n-1}, E_{n-1})$**, \(E \approx\) a computable contribution for the error in the adjoint arising from operator splitting

- **$Q_3$** is a noncomputable *a priori* expression that is provably higher order
Accuracy of the error estimate for the Brusselator example over $[0, 2]$
Accuracy of the error estimate for the Brusselator example at $T = 8$ and $T = 40$

![Graphs showing error for Species 1 and Species 2](image-url)
Conclusion
Conclusion

A posteriori error analysis based on duality, variational analysis, and adjoint equations provides a functional analytic approach to accurate computational error estimation.

Deriving the estimates and quantifying sources of discretization errors provides significant insight into the behavior of the numerical scheme.

Consideration of the adjoint problem provides insight into the stability, e.g., accumulation, propagation, and transmission of error.

Having accurate estimates not only is a key aspect of uncertainty quantification, but it also is useful for computation in several different ways.
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Limited References

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