Asymptotic Error Analysis - part I

Brian Wetton

Mathematics Department, UBC
www.math.ubc.ca/~wetton

National Chiao Tung University, December 6, 2010
Outline

Overview

Introductory Examples
  Romberg Integration
  DE example

Uses of Error Analysis
  Discrete Regularity
  Convergence Analysis of Nonlinear Problems
  Boundary Conditions

Higher Order Methods
  Cubic Splines
  Higher Order Difference Methods

Summary
Overview

• Errors from computational methods using regular grids to compute smooth solutions have additional structure.
• This structure can
  • allow Richardson Extrapolation
  • lead to super-convergence
  • help in the analysis of methods for non-linear problems
• Numerical artifacts (non-standard errors) can be present
• The process of finding the structure and order of errors is called Asymptotic Error Analysis (Herbert Keller).
• The method can be used to identify the order of accuracy of boundary condition implementation.
• Historical examples: Romberg Integration, “Strang’s Trick”, Cubic Splines.
• Need smooth solutions and regular grids.
Trapezoidal Rule

- Trapezoidal Rule $T_h$ approximation to $\int_a^b f(x)dx$ is the sum of areas of red trapezoids.
- Widths $h = (b - a)/N$ where $N$ is the number of sub-intervals.
- Error estimate
  $$\int_a^b f(x)dx - T_h = -\frac{(b - a)}{12} f''(\xi)h^2$$
- Second order convergence.
Trapezoidal Rule Applied

Trapezoidal Rule applied to the integral $I = \int_0^1 \sin x \, dx$

<table>
<thead>
<tr>
<th>$h$</th>
<th>$I - T_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>0.0096</td>
</tr>
<tr>
<td>1/4</td>
<td>0.0024</td>
</tr>
<tr>
<td>1/8</td>
<td>0.00060</td>
</tr>
<tr>
<td>1/16</td>
<td>0.00015</td>
</tr>
<tr>
<td>1/32</td>
<td>0.00004</td>
</tr>
</tbody>
</table>

Not only is

$$\int_a^b f(x) \, dx - T_h = - \frac{(b - a)}{12} f''(\xi) h^2$$

but $f''(\xi)$ in the expression tends to a constant value as $h \to 0$. There is regularity in the error that can be exploited.
Error Analysis of Trapezoidal Rule

- We had
  \[ \int_{a}^{b} f(x) \, dx - T_h = -\frac{(b - a)}{12} f''(\xi) h^2 \]

- but with a bit more work it can be shown that
  \[ \int_{a}^{b} f(x) \, dx - T_h = -\frac{1}{12} (f'(b) - f'(a)) h^2 + O(h^4) \]

- with more work the error in Trapezoidal Rule can be written as a series of regular terms with even powers of \( h \) (Euler-McLaurin Formula).
- This error regularity justifies Richardson extrapolation
  \[ \int_{a}^{b} f(x) \, dx - \left( \frac{4}{3} T_{h/2} - \frac{1}{3} T_h \right) = O(h^4) \]

- The \( O(h^4) \) error above is regular and so can also be eliminated by extrapolation. Repeated application of this idea is the Romberg method.
Interesting Facts

- Richardson extrapolation of the Trapezoidal Rule is Simpson’s Rule
- Trapezoidal and Midpoint Rules are spectrally accurate for integrals of periodic functions over their period
Example Problem
Find $u(x, t), t \geq 0, x \in [0, 2\pi]$, periodic in $x$ such that

$$
\begin{align*}
  u_t &= u_{xx} + f(x, t) \\
  f(x, t) &= e^{\cos x} \left( \cos t - \sin t[\sin^2 x - \cos x] \right) \\
  u(x, 0) &\equiv 0.
\end{align*}
$$

The exact solution is

$$
u(x, t) = e^{\cos x} \sin t$$
Discretization

- Divide $[0, 2\pi]$ into $N$ sub-intervals of length $h = 2\pi/N$. Let $U_i(t) \approx u(ih, t), \ i = 1 \cdots N$.

- Let $D_2$ be the second order centred finite approximation of the second derivative

\[
D_2 U_i = \frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = u_{xx}(ih, t) + \frac{h^2}{12}u_{xxxx}(ih, t) + O(h^4)
\]

- Semi-discrete scheme (method of lines):

\[
\frac{dU_i}{dt} = D_2 U_i + f(ih, t) \\
U_i(0) \equiv 0
\]
Convergence Proof
The error $E_i(t) = U_i(t) - u(ih, t)$ satisfies

\[
\begin{align*}
\frac{dU_i}{dt} &= D_2 U_i + f(ih, t) \\
\frac{du_i}{dt} &= D_2 u_i + f(ih, t) + t(ih, t) \\
\frac{dE_i}{dt} &= D_2 E_i - r(ih, t)
\end{align*}
\]

where (up to some fixed time $T$) the truncation error $r$ is bounded by $Ch^2$. We use mean square norm

\[
\|E\|_2 = \sqrt{h \sum_{i}^{N} E_i^2}
\]
Convergence (cont)

\[ \frac{dE_i}{dt} = D_2 E_i - r(ih, t) \]

Multiplying the equation above by \( h \) and taking the inner product with \( E \) gives (\( D_2 \) is negative definite)

\[ \frac{d\|E\|_2}{dt} \leq Ch^2 \]

or \( \|E(t)\|_2 \leq CTh^2 \) (convergence). This is a simple example of the Lax Equivalence Theorem (stability + consistency → convergence).
Numerical Convergence Study

- Error $E = U - u$.

- Second order scheme, have proved second order convergence $\|E_h\|_2 \leq Ch^2$.

- This is observed computationally in maximum norm in the error $\|E\|_\infty = \max_{i=1\ldots N} |E_i|$.

- The convergence rate is estimated as

$$\log_2 \frac{\|E_{2h}\|_\infty}{\|E_h\|_\infty}$$

<table>
<thead>
<tr>
<th>$N$</th>
<th>$|E|_\infty$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.0868</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.0198</td>
<td>2.1</td>
</tr>
<tr>
<td>32</td>
<td>0.0048</td>
<td>2.0</td>
</tr>
<tr>
<td>64</td>
<td>0.0012</td>
<td>2.0</td>
</tr>
</tbody>
</table>
Error Analysis The computational results above suggest that

\[ \| E_h \|_\infty \approx Ch^2 \]

with \( C \) independent of \( h \). Actually, we see this behaviour at every location \( x \):

\[ U_i(t) = u(ih, t) + h^2 e(ih, t) + O(h^4) \]

where \( e(x, t) \) is a smooth function independent of \( h \). It can be shown that \( e(x, t) \) solves

\[ e_t = e_{xx} - \frac{1}{12} u_{xxxx} \]

with \( e(x, 0) \equiv 0 \).
Error Analysis (cont.)

- $u(x, t) + h^2 e(x, t) + \cdots$ is an Asymptotic Error Expansion for the scheme.
- The first two terms above satisfy the discrete equations to fourth order accuracy. With more terms, the error expansion can satisfy the discrete equations to higher order.
- $e_t = e_{xx} - \frac{1}{12} u_{xxxx}$. The equations for the terms in the error expansion satisfy the original equations linearized around the exact solution, forced by lower order terms and their derivatives.
- **Note:** This is not the same as an equivalent equation approach.
Discrete Regularity
Our convergence proof is easily modified to show that

$$\| U - (u + h^2 e) \|_2 \leq Ch^4$$

Since $$\| U \|_\infty \leq \| U \|_2 / \sqrt{h}$$, we see that

$$\| U - (u + h^2 e) \|_\infty \leq Ch^{7/2}$$

and so

$$\| U - u \|_\infty \leq Kh^2$$

(for \( h \) sufficiently small).
Discrete Regularity (cont.)

Let $D_1$ be the second order centred difference approximation to the first derivative. Consider the convergence of $D_1 U$ to $u_x$ starting from

$$U = u + h^2 e + o(h^{7/2})$$

in maximum norm.

$$D_1 U = D_1 u + h^2 D_1 e + o(h^{5/2})$$

$$D_1 U = u_x + h^2 e_x + O(h^2) + o(h^{5/2})$$

That is, second order convergence in maximum norm of $D_1 U$ to $u_x$.

- This property of discrete solutions on regular grids is called super-convergence in the Finite Element community (but also other things are called super-convergence).
- Difference approximations to second and higher order derivatives also converge with second order.
Extrapolation

\[ U = u + h^2 e + O(h^4) \]

We can see that

\[ \frac{4}{3} U_h - \frac{1}{3} U_{2h} \]

(Richardson extrapolation) converges to \( u \) with fourth order.

If the exact solution of a problem is not known, the rate of convergence can be estimated using

\[
\log_2 \frac{\| U_{2h} - U_h \|_\infty}{\| U_h - U_{h/2} \|_\infty}
\]
Parameter Dependence If the PDE had a parameter $\mu$ then $U(\mu)$ depends smoothly on $\mu$ if the regular grid is held fixed:

$$U(\mu) = u(\mu) + h^2 e(\mu) + O(h^4)$$

This is especially important when sensitivities are estimated. Suppose $f(u)$ is a functional, approximated to second order by $F(U)$:

$$\frac{df(u(\mu))}{d\mu} = \frac{F(U(\mu + \Delta \mu)) - F(U(\mu + \Delta \mu))}{\Delta \mu} + O(h^2) + O(\Delta \mu).$$

Without error regularity, the errors above are $O(h^2/\Delta \mu)$. 
Strang’s Trick


• Suppose \( u(x, t), \, 0 \leq t \leq T, \, x \in [0, 1], \) periodic in \( x \) is smooth and solves \( u_t = f(u_x) \).

• Divide \([0, 1]\) into \( N \) sub-intervals of length \( h = 1/N \). Let \( U_i(t) \approx u(ih, t), \, i = 1 \cdot \cdot \cdot N \).

• Let \( D_1 \) be the second order centred finite approximation of the first derivative

\[
D_1 U_i = \frac{U_{i+1} - U_{i-1}}{2h} = u_x(ih, t) + \frac{h^2}{6} u_{xxx}(ih, t) + O(h^4)
\]

• Semi-discrete scheme (method of lines):

\[
\frac{dU_i}{dt} = f(D_1 U)
\]
Analysis of Scheme-I

\[ \frac{dU_i}{dt} = f(D_1 U) \]
\[ \frac{du_i}{dt} = f(D_1 u) - \frac{1}{6} f'(u_x) u_{xxx} h^2 + O(h^4) \]

Introduce the error \( E = U - u \)

\[ \frac{dE_i}{dt} = f'(D_1 u) D_1 E + f''(D_1 (u + \theta E))(D_1 E)^2 + O(h^2) \]

Introduce the discrete \( l_2 \) norm

\[ \| E \|_2 = \sqrt{h \sum_{i=1}^{N} E_i^2} \]

Note that

\[ \| E \|_\infty \leq h^{-1/2} \| E \|_2 \]
Analysis of the Scheme-II

To handle the nonlinear error, a bootstrap argument is used. Assume

$$\left\| E \right\|_2 \leq h^p \text{ for } t \leq T$$

and show that the scheme converges with order greater than $p$ to finish the argument.

$$\frac{dE_i}{dt} = f'(D_1 u)D_1 E + f''(D_1(u + \theta E))(D_1 E)^2 + O(h^2)$$

Multiplying the equation above by $h$ and taking the inner product with $E$ gives (after summation by parts)

$$\frac{d\left\| E \right\|_2}{dt} \leq \left\| Df'(D_1 u) \right\|_\infty \left\| E \right\|_2 + \left\| f''(D_1(u + \theta E)) \right\|_\infty h^{p-5/2} \left\| E \right\|_2 + O(h^2)$$

Note that the bootstrap argument can’t be closed with this estimate.
Asymptotic Error Analysis-I

The truncation error is smooth so it is reasonable to expect error regularity

\[ U = u + h^2 e + O(h^4) \]

with \( e \) a smooth function of \( x \) and \( t \), independent of \( h \). I’ll show how to construct this function \( e \) below, but assume it exists:

- \( u + h^2 e \) has truncation error \( O(h^4) \) in the discrete equations so by using \( E = U - (u + h^2 e) \) in the analysis above, the bootstrap argument can be closed.

- The error expression above can be used to show full order convergence in maximum norm and difference approximations to derivatives (super-convergence)

\[ D_2 U = u_{xx} + h^2 \left( \frac{1}{12} u_{xxxx} + e_{xx} \right) + O(h^4) \]

- Error regularity also leads to full order convergence of derivatives of solution functionals with respect to parameters.
Asymptotic Error Analysis-II

- Want $u + h^2 e$ to satisfy the discrete equations

$$\frac{dU}{dt} = f(D_1 U)$$

to fourth order.

- Plug in, expand, identify the $O(h^2)$ term:

$$e_t = f'(u_x) e_x + \frac{1}{6} f'(u_x) u_{xxx}$$

- Realize that this problem (linearization about the exact solution forced by terms involving derivatives of the exact solution) has a smooth solution. You don’t have to find the solution, just know that it exists.
Convergence of Nonlinear Problems (cont.)

- For problems with nonlinearities in derivatives of order $m$ in $n$ dimensions we would need convergence of order $2m + n/2$ in $\| \cdot \|_2$ norm for this argument.

- We can get arbitrarily high order accuracy to an asymptotic error expansion with enough terms, making this argument possible.
More History

New Model Problem
Find $u(x, t), \ t \geq 0, \ x \in [0, 1]$ with
\[
\begin{align*}
  u_t &= u_{xx} + f(x, t) \\
  u(x, 0) &= 0 \\
  u_x(0, t) &= g(t) \\
  u(1, t) &= 0
\end{align*}
\]

Divide $[0, 1]$ into $N$ subintervals of length $h = 1/N$. Let $U_i(t) \approx u(ih, t), \ i = 0 \ldots N - 1$.
\[
\frac{dU_i}{dt} = D_2 U_i + f(ih, t)
\]
A value of $U_{-1}$ is needed to complete the discrete problem.
Ghost Points

- A value of $U_{-1}$ is needed to complete the discrete problem and the boundary condition $u_x(0, t) = g(t)$ has not been implemented.

- A second order approximation at the boundary is

$$D_1 U_0 = g(t), \quad \text{error } \frac{h^2}{6} u_{xxx}(0, t)$$

which can be rewritten $U_{-1} = U_1 - 2hg(t)$.

- This can be implemented as an algebraic condition in the discrete problem or it can be used to eliminate $U_{-1}$ from the interior discretization.
Error Analysis

- As before, the discrete scheme has an error expansion
  \[ U = u + h^2 e + \cdots. \]
- Here, \( e \) solves \( e_t = e_{xx} - \frac{1}{12} u_{xxxx} \) with \( e(x,0) \equiv 0 \) as before but now \( e(1, t) = 0 \) and
  \[ e_x(0, t) = -\frac{1}{6} u_{xxx}(0, t) \]
- Note that
  \[ D_2 U_0 = \frac{2(U_1 - U_0) - 2hg(t)}{h^2} \]
is formally only first order accurate to the exact solution. Because of the higher order terms in the error expansion, computed values of \( D_2 U_0 \) will be second order accurate (for \( t > 0 \), there can be incompatibilities in the initial data that limit the convergence at \( t = 0 \) that are smoothed out at later times).
Error Analysis (cont.)

- Formally first order accurate:

\[ D_2 U_0 = \frac{2(U_1 - U_0) - 2hg(t)}{h^2} \]

- There is a lot of confusion on this point in the literature. There is a common misconception that the (incorrect) rule, “the discretized operator near the boundary can be one order lower”, applies.

- For smooth problems, the accuracy at which the boundary condition is approximated determines the accuracy of the scheme.
General Boundary Conditions

- The Robin condition $u_x(0, t) = \alpha u(0, t) + g(t)$ is approximated by $D_1 U_0 = \alpha U_0 + g$ or $U_{-1} = U_1 - 2h(\alpha U_0 + g)$.
- For staggered (by $h/2$) grids $u_x(0, t)$ is approximated to second order by $(U_{1/2} - U_{-1/2})/h$.
- On staggered grids $u(0, t)$ is approximated to second order by $(U_{1/2} + U_{-1/2})/2$.
- For (almost) all well-posed parabolic systems, mixed Dirichlet-Neumann conditions can be implemented using the staggered grid ghost point approximations above.
Triple Junctions

In the application, three curves (described by second order parabolic equations in two coordinates with a parameter \( \sigma \)) meet at a common point with symmetric (120°) angles.
Triple Junctions (cont.) If $\sigma = 0$ is the triple junction then

\[
x^{(1)}(0, t) = x^{(2)}(0, t) = x^{(3)}(0, t)
\]

\[
t^{(1)} + t^{(2)} + t^{(3)} = 0
\]

(6 conditions) where $t^{(i)}$ is the tangent vector of curve $i$ at $\sigma = 0$. These conditions can be easily implemented on a staggered grid by

\[
X_{1/2}^{(1)} + X_{-1/2}^{(1)} = X_{1/2}^{(2)} + X_{-1/2}^{(2)} = X_{1/2}^{(3)} + X_{-1/2}^{(3)}
\]

\[
T^{(1)} + T^{(2)} + T^{(3)} = 0
\]

where

\[
T^{(i)} = \frac{X_{1/2}^{(i)} - X_{-1/2}^{(i)}}{|X_{1/2}^{(i)} - X_{-1/2}^{(i)}|}
\]

These relationships for the ghost values $X_{-1/2}^{(i)}$ become part of the implicit solve when implicit time stepping is used.
Cubic Splines

- Given smooth $f(x)$ on [0,1], spacing $h = 1/N$, and data $a_i = f(ih)$ for $i = 0, \ldots, N$ the standard cubic spline fit is a $C_1$ piecewise cubic interpolation.
- Cubic interpolation on each sub-interval for given values and second derivative values $c_i$ at the end points is fourth order accurate.
- If the second derivative values are only accurate to second order, the cubic approximation is still fourth order accurate.
- For $C_1$ continuity,
\[
c_{i-1} + 4c_i + c_{i+1} = \frac{6}{h^2}(a_{i+1} - 2a_i + a_{i-1})
\]
Cubic Splines - Periodic Analysis

\[ c_{i-1} + 4c_i + c_{i+1} = \frac{6}{h^2}(a_{i+1} - 2a_i + a_{i-1}) \]

In this case, \( c \) has a regular asymptotic error expansion

\[ c = f'' + h^2\left(\frac{1}{12} - \frac{1}{6}\right)f'''' + \ldots \]

(the fact that \( c_{i-1} + c_{i+1} = 2c_i + h^2c'' + \ldots \) is used). Since the \( c \)'s are second order accurate, the cubic spline approximation is fourth order accurate.

Notes:

- The earliest convergence proof for splines is in this equally spaced, periodic setting Ahlberg and Nilson, “Convergence properties of the spline fit”, J. SIAM, 1963
Cubic Splines - Non-Periodic Case

\[ c_{i-1} + 4c_i + c_{i+1} = \frac{6}{h^2}(a_{i+1} - 2a_i + a_{i-1}) \]

In the non-periodic case, additional conditions are needed for the end values \( c_0 \) and \( c_N \):

- **natural:** \( c_0 = 0, \, O(1) \)
- **derivative:** \( 2c_0 + c_1 = \frac{6}{h^2}(a_1 - a_0) - \frac{3}{h}f'(0), \, O(h^2) \)
- **not a knot:** \( c_0 - 2c_1 + c_2 = 0, \, O(h^2) \)

Cubic Splines - Numerical Boundary Layer

\[ c_{i-1} + 4c_i + c_{i+1} = \frac{6}{h^2}(a_{i+1} - 2a_i + a_{i-1}) \]

No regular error can match the natural boundary condition \( c_0 = 0 \). However, note that

\[ 1 + 4\kappa + \kappa^2 = 0 \]

has a root \( \kappa \approx -0.268 \).

Error Expansion:

\[ c_i = f''(ih) - h^2 \frac{1}{6} f''''(ih) - f''(0)\kappa^i \ldots \]

The new term is a numerical boundary layer. In this case, the spline fit will be second order near the ends of the interval and fourth order in the interior. Reference?
Cubic Splines - Computation
Compact Scheme Start with

\[ u_t = u_{xx} + f(x, t). \]

The second order scheme \( \dot{U} = D_2 U + f(x, t) \) has errors \( \frac{h^2}{12} u_{xxxx} \).

By taking two derivatives of the equation above we see that

\[ u_{xxxx} = u_{txx} - f_{xx} \]

Therefore the scheme

\[ (I - \frac{h^2}{12} D_2) \dot{U} = D_2 U + (I - \frac{h^2}{12} D_2) f \]

will be fourth order accurate with regular errors (if all boundary conditions are approximated to fourth order accuracy). Implicit time stepping is natural for this method.
Wide Scheme Another fourth order scheme for \( u_t = u_{xx} + f(x, t) \) is

\[
\dot{U} = \tilde{D}_2 U + f
\]

where \( \tilde{D}_2 = D_2(I - \frac{h^2}{12} D_2) \) is the fourth order accurate centred difference operator for the second derivative.

- Note that \( \tilde{D}_2 \) requires values of \( U \) up to 2 grid points away.
- When a Dirichlet condition \( u(0, t) = 0 \) is specified, the ghost point \( U_{-1} \) is still needed. An artificial condition must be specified.
- Use \( D_4 U_1 = 0 \) (equivalent to fourth order extrapolation of interior values to \( U_{-1} \)).
Error Analysis of Wide Scheme

\[ \dot{U} = \tilde{D}_2 U + f \]

With \( U_0 = 0 \) and \( D_4 U_1 = 0 \). The error expansion for this scheme is

\[ U_i(t) \approx u(ih, t) + h^4 e(ih, t) + h^4 A(t)\kappa^i + \cdots \]

where \( e \) is smooth and \( \kappa \approx 0.072 \) are independent of \( h \).

- The last term above is a numerical boundary layer at \( x = 0 \). There is a similar boundary layer at \( x = 1 \) not shown.
- \( \kappa \) is a root of \( (I - \frac{h^2}{12} D_2)\kappa^i = 0 \). The roots come in reciprocal pairs.
- The boundary conditions \( U_0 = 0 \) and \( D_4 U_1 = 0 \) are matched to high order by choice of \( A \) and \( e(0, t) \).
- The convergence rate of difference approximations near the boundary (only) is limited by the numerical boundary layer.
- Approximation by cubic splines also has similar boundary layer effects.
Summary

- Asymptotic error analysis can be used to describe regular errors and numerical artifacts in finite difference methods and other schemes on regular meshes.
- This error analysis can be used to
  - justify discrete regularity and extrapolation.
  - aid in the convergence proof of methods for nonlinear problems
  - identify the order and type of errors coming from the approximation of boundary conditions.
- Historical examples of Romberg integration; finite difference approximations of nonlinear, first order equations; and spline interpolation were given.