Asymptotic Error Analysis

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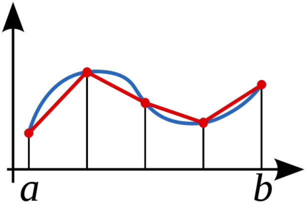
- Faculty participation from many departments.
- Interdisciplinary graduate programme.

Overview of the Talk

- Errors from computational methods using regular grids to compute smooth solutions have additional structure.
- This structure can
  - allow Richardson Extrapolation
  - lead to super-convergence
  - guide the implementation of boundary conditions
  - 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 can be called Asymptotic Error Analysis. Needs smooth solutions and regular grids.
- Historical examples: Romberg Integration and Cubic Splines
- New result: a numerical artifact from an idealized adaptive grid with hanging nodes.

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 bound

$$\left| \int_a^b f(x)dx - T_h \right| \leq \frac{(b-a)}{12} K h^2$$

where $K = \max |f''|$
- Second order convergence.

Proof of Error Bound-I

- Consider a subinterval $x \in [0, h]$.
- Let $L(x)$ be linear interpolation on this subinterval and $g(x) = f(x) - L(x)$, so $g(0) = g(h) = 0$.
- The error E of trapezoidal rule on this subinterval is

$$E = \int_0^h g(x)dx$$

- Integrate by parts twice

$$\begin{aligned} E &= -\int_0^h (x - h/2)g'(x)dx \\ &= \frac{1}{2}\int_0^h (x^2 - xh)g''(x)dx = \frac{1}{2}\int_0^h (x^2 - xh)f''(x)dx \end{aligned}$$

Proof of Error Bound-II

Subinterval $E = \frac{1}{2}\int_0^h (x^2 - xh) f''(x) dx$

$$|E| \leq \frac{K}{2}\int_0^h (xh - x^2) dx = \frac{Kh^3}{12}.$$

Summing over $N = (b-a)/h$ subintervals gives the result

$$|I - T_h| \leq \frac{(b-a)}{12} Kh^2$$

Trapezoidal Rule Applied

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

h	$I - T_h$
1/2	0.0096
1/4	0.0024
1/8	0.00060
1/16	0.00015
1/32	0.00004

Not only is

$$|I - T_h| \leq \frac{(b-a)}{12} K h^2$$

but

$$\lim_{h \to 0} \frac{I - T_h}{h^2}$$

exists. There is *regularity* in the error that can be exploited.

Error Analysis of Trapezoidal Rule-I

- We had
$$|E| \leq \frac{Kh^3}{12} \Rightarrow |I - T_h| \leq \frac{(b-a)}{12} Kh^2$$
- but with a bit more work it can be shown that
$$\begin{aligned} E &= -f''_{ave} h^3/12 + O(h^5) \Rightarrow \\ I - T_h &= -\frac{(b-a)}{12} Ch^2 + O(h^4) \end{aligned}$$
  where C is average value of f'' on the subinterval.
- 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).

Error Analysis of Trapezoidal Rule-II

$$T_h = I + \frac{(b-a)}{12} C h^2 + O(h^4)$$

- This error regularity justifies Richardson extrapolation

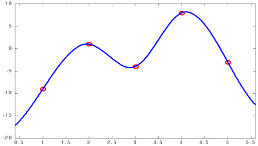
$$I = (\frac{4}{3} T_{h/2} - \frac{1}{3} T_h) + O(h^4)$$

- 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

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

$$c = f'' + h^2(\frac{1}{12} - \frac{1}{6})f'''' + \ldots$$

(the fact that $c_{i-1} + c_{i+1} = 2c_i + h^2 c'' + \ldots$ 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
- Lucas, "Asymptotic expansions for interpolating periodic splines," SINUM, 1982.

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: $c_0 - 2c_1 + c_2 = 0,\ O(h^2)$

First convergence proof for "derivative" conditions Birkhoff and DeBoor, "Error Bounds for Spline Interpolation", J Math and Mech, 1964.

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

$$1 + 4\kappa + \kappa^2 = 0$$

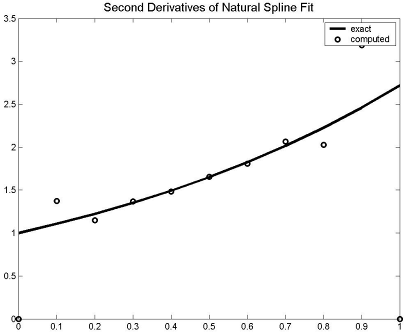
has a root $\kappa \approx -0.268$.

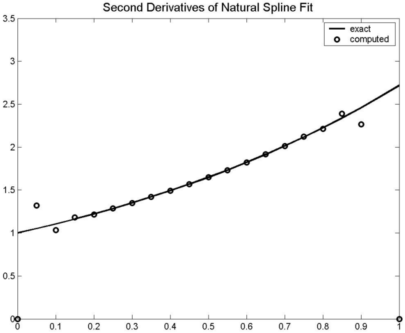
Error Expansion:

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

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





More History

- Strang, "Accurate Partial Differential Methods II. Non-linear Problems," Numerische Mathematik, 1964
- Goodman, Hou and Lowengrub, "Convergence of the Point Vortex Method for the 2-D Euler Equations," Comm. Pure Appl. Math, 1990
- E and Liu, "Projection Method I: Convergence and Numerical Boundary Layers," SINUM, 1995

1D Boundary Value Problem

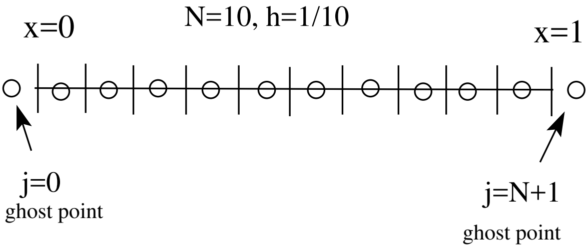
Simple boundary value problem for $u(x)$:

$$u'' - u = f \quad \text{with } u(0) = 0 \text{ and } u(1) = 0$$

with f given and smooth.

Theory: Unique solution $u \in C^{k+2}$ for every $f \in C^k$.

- N subintervals, spacing $h = 1/N$.
- Cell-Centred Finite Difference approximations $U_j \approx u((j-1/2)h, j = 0 \ldots N+1$.



Uniform Grid

Scheme

$$u'' - u = f \quad \text{with } u(0) = 0 \text{ and } u(1) = 0$$

- Finite Difference approximation for interior grid points

$$\frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} - U_j = f(jh)$$

  truncation error $h^2 u''''(jh)/12 + O(h^4)$.

- Linear Interpolation of the boundary conditions

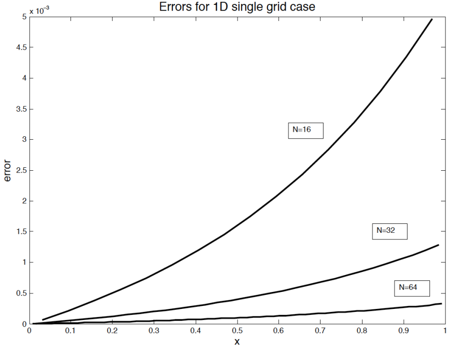
$$\frac{U_0 + U_1}{2} = 0$$

  truncation error $h^2 u''(0)/8 + O(h^4)$.

Lax Equivalence Theorem: A stable, consistent scheme converges with the order of its truncation error.

Uniform Grid

Computational Results



Note that: the computed $U = u + h^2 u^{(2)} + O(h^4)$ with $u^{(2)}$ a smooth function of x. This is an asymptotic error expansion for U with only regular terms (no artifacts).

Uniform Grid

Asymptotic error expansion

$$U = u + h^2 v(x) + O(h^4)$$

$$\begin{aligned} \frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} - U_j &= f(jh) + h^2 u''''(jh)/12 + O(h^4) \\ \frac{U_0 + U_1}{2} &= h^2 u''(0)/8 + O(h^4) \end{aligned}$$

Match terms at $O(h^2)$:

$$v'' - v = u''''/12 \quad \text{with } v(0) = u''(0)/8 \text{ and } v(1) = u''(1)/8$$

Error solves the original DE but with truncation error data.
Note: v is just a theoretical tool. Justifies full order convergence of derivative approximations (super-convergence):

$$(U_{j+1} - U_{j-1})/(2h) = u_x(jh) + O(h^2)$$

Uniform Grid

Be careful on interpreting BC accuracy

At the boundary we have

$$\frac{U_0 - 2U_1 + U_2}{h^2} - U_j = f(0) \quad \text{and} \quad \frac{U_0 + U_1}{2} = 0$$

These can be combined to give

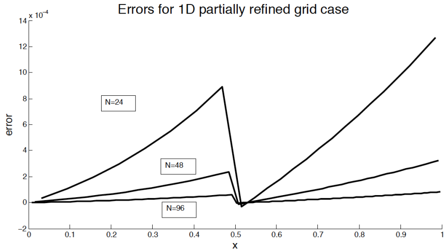
$$\frac{-3U_1 + U_2}{h^2} - U_j = f(0)$$

which is not consistent (errors do not $\to 0$ as $h \to 0$).

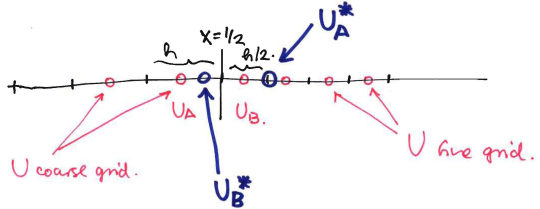
Interpret BC accuracy in discrete approximations of the original accuracy

1D Partially Refined Grid

- Refine the grid in the right half of the interval by a factor of 2.
- Ghost points at the refinement interface are related to grid values by linear interpolation/extrapolation.
- Second order convergence is seen in the solution.
- The computed U has a piecewise regular error expansion.



1D Partially Refined Grid Analysis



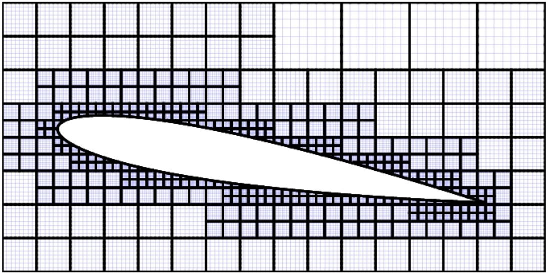
- Linear interpolation $U_B^* = \frac{2}{3} U_A + \frac{1}{3} U_B$
- Linear extrapolation $U_A^* = -\frac{1}{3} U_A + \frac{4}{3} U_B$
- Determine the accuracy at which the "interface" conditions $[u] = 0$ and $[u'] = 0$ are approximated.
- The conditions above can be rewritten as

$$\begin{aligned} (U_A + U_A^*)/2 &= (U_B + U_B^*)/2 \\ (U_A^* - U_A)/h &= (U_B - U_B^*)/(h/2) \end{aligned}$$

so are second order approximations of the interface conditions.

Piecewise Regular Grids

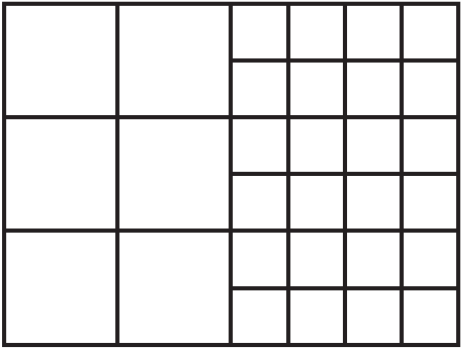
- Computations on regular grids have many advantages.
- To retain some of the advantages but allow adaptivity, refinement in regular blocks is often done.



Clinton Groth, University of Toronto

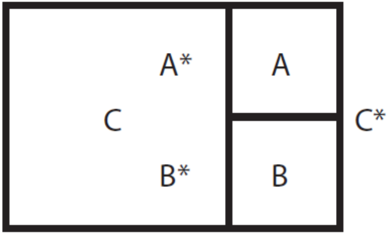
Idealized Piecewise Regular Grid

Consider the idealized setting of a coarse grid and fine grid with a straight interface:

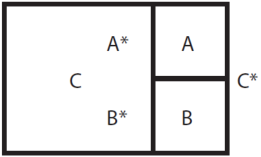


Problem and Discretization

- Consider the problem $\Delta u = f$.
- The grid spacing is h (coarse) and $h/2$ (fine).
- The discrete approximation is cell-centred, denoted by U.
- Away from the interface, a five point stencil approximation is used.
- At the interface, ghost points are introduced, related to grid points by linear extrapolation.



Analysis of Piecewise Regular Grid-II



- The ghost point extrapolation is equivalent to

$$\begin{aligned} \frac{1}{4}(U_A + U_{A*} + U_B + U_{B*}) &= \frac{1}{2}(U_C + U_{C*}) \\ \frac{1}{h}(U_A - U_{A*} + U_B - U_{B*}) &= \frac{1}{h}(U_{C*} - U_{C*}) \\ (U_A - U_B - U_{A*} + U_{B*}) &= 0 \end{aligned}$$

- The first two conditions are second order approximations of the "interface" conditions $[u] = 0$ and $[\partial u/\partial n] = 0$.
- They contribute to the second order regular errors of the scheme (different on either side of the grid interface).

Analysis of Piecewise Regular Grid-III

$$(U_A - U_B - U_{A*} + U_{B*}) = 0$$

- This is satisfied to second order by the exact solution, error $h^2 u_{xy}/4$.
- Note that this only involves fine grid points.
- Expect a parity difference between fine grid solutions at the interface.
- This results in a numerical artifact of the form

$$h^2 A(y)(-1)^j \kappa^i$$

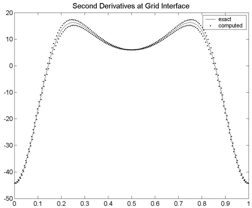
  where (i, j) is the fine grid index and $\kappa \approx 0.172$.
- This is a numerical boundary layer on the fine grid side that alternates in sign between vertically adjacent points.

Piecewise Regular Grid - Analysis Summary

- Coarse grid has regular error $U_{coarse} = u + h^2 e_{coarse} + \ldots$
- Fine grid has regular error and the artifact

$$U_{fine} = u + h^2 e_{fine} + h^2 \frac{u_{xy}(0, y)}{8(1-\kappa)} (-1)^j \kappa^i + \cdots$$

- Artifact causes loss of convergence in $D_{2,y} U$ and $D_{2,x} U$ *on the fine grid side at the interface.*



Additional Discussion

$$h^q A(y)(-1)^j \kappa^i$$

- This artifact is present in all schemes (FE, FD, FV) on the grid, although the q may vary.
- Determinant condition, satisfied for stable schemes.
- For variable coefficient elliptic problems, $\kappa(y)$ smooth.

Summary

- Asymptotic error analysis can be used to describe regular errors and numerical artifacts in finite difference methods and other schemes on regular meshes.
- Historical examples of Romberg integration and spline interpolation were given.
- Asymptotic error analysis can be used to help understand the accuracy of different implementations of boundary and interface conditions.
- A new result describing the errors in methods for elliptic problems on piecewise regular grids with hanging nodes was given.