Finite difference methods, Green functions and error analysis, IB/IIM methods

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Online, 2021

Lecture 1

- Finite difference basics
- References
  - Numerical Solution of Differential Equations – Introduction to Finite Difference and Finite Element Methods, Cambridge University Press, 2017.
  - Some papers
  - Matlab Codes: https://zhilin.math.ncsu.edu/TEACHING/MA584/index.html
- Course Delivery Method: Classes will be delivered online during the class time using Zoom. The classes will be recorded. The video and notes will be available.

  Note that: In case of possible Internet outages, please wait up to for 5 minutes or so to get reconnected.

Introduction

- Differential Equations (ODE/PDEs)
  - Initial value problems (IVPs)
  - Boundary value problems (BVPs)
  - Initial and boundary value problems, have to be time dependent
- Classification of ODE/PDEs
  - Mathematical: order, linearity (quasi-linear), constant/variable coefficient(s), homogeneity/source terms
  - Physical: advection, heat, wave, elliptic equations; Laplace/Poisson equations
  - Hyperbolic, elliptic*, parabolic* (compare with quadratic curves)
- Well-posedness of ODE/PDES, existence, uniqueness, and sensitivity
- Solution techniques Analytic: PDE convert to ODE Approximate semi-analytic; numerical solutions

FDM for IVP problems, Matlab ODE-Suite

- Canonical form (no space derivative)

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}\left(t, \mathbf{y}\right), \qquad \mathbf{y}(t_0) = \mathbf{v}, \tag{1}$$

- Well-posed if **f** is Lipschitz continuous.

$$\begin{aligned}
\frac{dy_1}{dt} &= f_1\left(t, y_1(t), y_2(t), \cdots, y_m(t)\right), \\
\frac{dy_2}{dt} &= f_2\left(t, y_1(t), y_2(t), \cdots, y_m(t)\right), \\
\vdots \quad & \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\
\frac{dy_m}{dt} &= f_m\left(t, y_1(t), y_2(t), \cdots, y_m(t)\right),
\end{aligned} \tag{2}$$

- High order would be converted to the standard form if possible.
- ode23, ode15s, ode45, etc. Useful for method of lines (MOL)
- FDM, forward/backward/central Euler method, Crank-Nicholson, Runge-Kutta, adaptive time steps etc.

Finite difference methods vs Finite element methods

Finite difference methods

- Long history. Simple and intuitive for regular domains (research for arbitrary ones)
- Point-wise discretization, error measure in the infinity norm
- Strong form
- Easier to obtain approximate derivatives with the same order of accuracy as the solution
- Compact and local, fast solvers, structured meshes
- Difficult for arbitrary geometry, smaller group
- Hard to prove the convergence
- Finite volume (FV) methods are special types of FDM.

Finite difference methods vs Finite element methods

Finite element methods, short history (1950-60's)

- Based on integral forms, testing function spaces and solution spaces. The solution is approximate by simple, piecewise functions
- Weak form, 2nd to first, 4th to second
- Lower order accuracy for derivatives, posterior error analysis
- Solid theoretical foundations based on Sobolev theory, Lax-Milgram, Lax-Milgram-Breeze
- Used to prove wellposedness of models
- Natural for mechanical problems
- Natural for general geometries but need expert knowledge in programming except for structure meshes.

Finite difference basics

Key: representing derivative(s) using combination of function values on grid points (finite)

- Basic finite difference formulas and **Operator notation**

$$
\begin{aligned}
\text{Forward :} \qquad & \Delta_+ u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h} = u'(\bar{x}) + O(h) \\
\text{Backward :} \qquad & \Delta_- u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h} = u'(\bar{x}) + O(h) \\
\text{Central :} \qquad & \delta u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = u'(\bar{x}) + O(h^2)
\end{aligned}
$$

- Discretization, discretization error, order of discretization
- **Q:** Can we take h arbitrarily small?

Finite difference formula for second order derivatives

- Central

$$
\begin{aligned}
\delta^2 u(\bar{x}) &= \frac{u(\bar{x}-h) - 2u(\bar{x}) + u(\bar{x}+h)}{h^2} = u''(\bar{x}) + O(h^2) \\
&= \Delta_+ \Delta_- u(\bar{x}) + O(h^2)
\end{aligned}
$$

- One-sided

$$
\Delta_+ \Delta_+ u(\bar{x}) = \frac{u(\bar{x}) - 2u(\bar{x}+h) + u(\bar{x}+2h)}{h^2} = u''(\bar{x}) + O(h)
$$

$$
\Delta_- \Delta_- u(\bar{x}) = \frac{u(\bar{x}-2h) - 2u(\bar{x}-h) + u(\bar{x})}{h^2} = u''(\bar{x}) + O(h)
$$

- **Q:** Do we have high order FD discretizations (Consider, the number of points, whether it is compact etc.)

Process of a finite difference method, notations

Use the example (when is it wellposed):

$$u''(x) = f(x), \quad a < x < b, \quad u(a) = u_a, \quad u(b) = u_b,$$

If $f(x) \in C(a,b)$, then $u(x) \in C^2(a,b)$ (FEM: if $f(x) \in L^2(a,b)$, then $u(x) \in H^2(a,b)$.

- Generate a grid, e.g. a uniform grid

$$x_i = a + i\,h, \quad i = 0, 1, \cdots n, \quad h = \frac{(b-a)}{n}, \quad x_0 = a, \quad x_n = b,$$

  with n being a parameter (control accuracy). x_i's are called grid points.

- At every grid point where the solution is unknown, substitute the DE with a finite difference approximation

$$u''(x_i) = \frac{u(x_i - h) - 2u(x_i) + u(x+h)}{h^2} + \frac{u^{(4)}(\xi_i)}{12}\,h^2 = f(x_i)$$

The $T_i = \frac{u^{(4)}(\xi_i)}{12} h^2$ is called the local truncation error (unknown).

- The finite difference solution (if exists) is defined as the solution of

$$
\begin{aligned}
\frac{u_a - 2U_1 + U_2}{h^2} &= f(x_1) \\
\frac{U_1 - 2U_2 + U_3}{h^2} &= f(x_2) \\
\cdots\cdots &= \cdots \\
\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} &= f(x_i) \\
\cdots\cdots &= \cdots \\
\frac{U_{n-3} - 2U_{n-2} + U_{n-1}}{h^2} &= f(x_{n-2}) \\
\frac{U_{n-2} - 2U_{n-1} + u_b}{h^2} &= f(x_{n-1}).
\end{aligned}
$$

So $U_i \approx u(x_i)$. How large/small is the difference? Need error analysis.

For this ODE, after finite difference, the problem becomes a linear system of equations $A_h U = F$, A_h is called discrete Laplacian,

$$\begin{bmatrix} -\frac{2}{h^2} & \frac{1}{h^2} & & & & \\ \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} \\ & & & & \frac{1}{h^2} & -\frac{2}{h^2} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_{n-2} \\ U_{n-1} \end{bmatrix} = \begin{bmatrix} f(x_1) - \frac{u_a}{h^2} \\ f(x_2) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) - \frac{u_b}{h^2} \end{bmatrix}$$

A_h is tridiagonal, symmetric, $-A_h$ is an SPD, an M-matrix

- The diagonals have one sign, all off-diagonals have opposite sign
- It's (weakly diagonally) row/column dominant, at least one row is strictly, irreducible
- Fast solver, chase method, $O(5N)$ complexity.

A_h is invertible. The system of the FD equations has a uniques solution.

Convergence analysis: Need consistency & stability

Convergence: $\lim_{h \to 0} |u(x_i) - U_i| = 0$ for all i's. Better to use $\lim_{h \to 0} \|\mathbf{u} - \mathbf{u}\| = 0$ in some norm, which one? $\|\cdot\|_\infty$, $\|\cdot\|_{L^2}$. **Called global error!**

Theorem: If a FDM is consistent & stable, then it is convergent. (A sufficient condition!)

- Consistency often is easy, $\lim_{h \to 0} T_i = 0$. $\|DE - FD\|_{\Omega_h} \to 0$. May have different expressions. Should use the correct one!
- **Stability** is often challenging for both FDM and FEM (sup-inf condition). Not many people pay attention to elliptic problems. Require: $\|A_h\| \le C$ so that the global error has the same order as the discretization, no deterioration in accuracy!

An example of consistency but no stability

If we use a consistent first order, one-sided FD formula at x_1

$$\frac{U_1 - 2U_2 + U_3}{h^2} = f(x_1)$$

What will happen? We have $T_1 \sim O(h)$ so it's consistent, but $det(A_1) = 0$ and there is no unique solution to $A_1 U = F$. The BC is not used!

The FD method fails!

Convergence proof and the optimal error estimate

The **global error** vector $\mathbf{E} = \mathbf{u} - \mathbf{U}$.

$$A_h \mathbf{u} = \mathbf{F} + \mathbf{T}, \; A_h \mathbf{U} = \mathbf{F} \implies A_h (\mathbf{u} - \mathbf{U}) = \mathbf{T} = -A_h \mathbf{E}, \; \mathbf{E} = A_h^{-1} \mathbf{T}.$$

We know $\|\mathbf{T}\|_\infty \le Ch^2$, but it's not so easy to estimate $\|A_h^{-1}\mathbf{T}\|$!

- Use eigenvalues of A_h. (R. LeVeque)
- Use discrete Green functions.
- Use a comparison function. (Morton & Mayers, J. H. Bramble)

Use eigenvalues of A_h

Explicit expression for tridiagonal matrices (α, d, α)

$A = full(gallery('tridiag', n, -1, 2, -1))/h^2$
Eigenvalues and eigenvectors

$$\lambda_j = -2 + 2\cos\frac{\pi j}{n}, \quad j = 1, 2, \cdots n-1,$$

$$x_k^j = \sin\frac{\pi kj}{n}, \quad k = 1, 2, \cdots n-1.$$

$$\|A_h\|_2 = \frac{2}{h^2}\left(1 - \cos\frac{\pi int(n/2)}{n}\right) \sim \frac{2}{h^2}$$

$$\|{A_h}^{-1}\|_2 = \frac{1}{\min|\lambda_j|} = 2\left(1 - \cos\frac{\pi}{n}\right) \sim \frac{1}{\pi^2}$$

$$cond_2(A_h) = \|A_h\|_2\|A_h^{-1}\|_2 \sim 4n^2$$

Large if n is large!

Error estimate using eigenvalues

Using the inequality $\|A_h^{-1}\|_\infty \le \sqrt{n-1}\,\|A_h^{-1}\|_2$, we have

$$\begin{aligned} \|\mathbf{E}\|_\infty &\le \|A_h^{-1}\|_\infty\,\|\mathbf{T}\|_\infty \le \sqrt{n-1}\,\|A_h^{-1}\|_2\,\|\mathbf{T}\|_\infty \\ &\le \frac{\sqrt{n-1}}{\pi^2}\,Ch^2 \le \bar{C}h^{3/2}, \end{aligned}$$

A decent estimate but not optimal. Expect to have $O(h^2)$!

Discrete Green function

Consider one error component E_i

$$E_i = \sum_{k=1}^{N-1} \left(A_h^{-1}\right)_{ik} T_k = h \sum_{k=1}^{N-1} \left(A_h^{-1}\right)_{ik} T_k \frac{1}{h} \mathbf{e}_k = h \sum_{k=1}^{N-1} T_k \left(A_h^{-1}\right)_{ik} \frac{1}{h} \mathbf{e}_k$$

Definition of discrete Green function in 1D:

$$G\left(x_i, x_l\right) = \left(A_h^{-1} \mathbf{e}_l \frac{1}{h}\right)_i, \qquad G\left(x_0, x_l\right) = 0, \quad G\left(x_n, x_l\right) = 0. \quad (3)$$

Analogue to a continuous problem

$$g''(x) = \delta(x - x_i), \qquad g(a) = 0, \quad g(b) = 0. \quad (4)$$

The solution is:

$$g(x, x_i) = \begin{cases} (b - x_i)x, & a < x < x_i, \\ (b - x)x_i, & x_i < x < b. \end{cases} \quad (5)$$

Discrete Green function II

- $G(x_i, x_l) = g(x_i, x_l)$, may not be true in 2D.
- Symmetry $G(x_i, x_l) = G(x_l, x_i)$.
- $O(1/h)$ at one point $\Longrightarrow$ $O(1)$ globally!
- 2D, $g = \log r$, 3D, $g = \frac{1}{r}$, discrete with different BC's.

$$E_i = \sum_{k=1}^{N-1} \left(A_h^{-1}\right)_{ik} T_k = h \sum_{k=1}^{N-1} \left(A_h^{-1}\right)_{ik} T_k \frac{1}{h} \mathbf{e}_k = h \sum_{k=1}^{N-1} T_k \left(A_h^{-1}\right)_{ik} \frac{1}{h} \mathbf{e}_k$$

$$\begin{aligned} |E_i| &= \left| h \sum_{k=1}^{N-1} T_k \left(A_h^{-1}\right)_{ik} \frac{1}{h} \mathbf{e}_k \right| \le \left| C h^3 \sum_{k=1}^{N-1} G(x_i, x_k) \right| \\ &\le C h^2 (b-a) \max\{|a|, |b|\}, \qquad C = \frac{u_{xxxx}}{12}. \end{aligned}$$

Which ones can you solve, or solve accurately?

- Pure Neumann BC

$$u''(x) = f(x), \quad a < x < b,$$
$$u'(a) = \alpha, \qquad u'(b) = u_b\,,$$

- **Periodic BC:** $u''(x) = f(x)$, $a < x < b$, What does it mean? $u(a) = u(b)$, $u'(a) = u'(b)$.
- How about this one?

$$u''(x) + u(x) = f(x), \quad 0 < x < \pi,$$
$$u(a) = 0, \qquad u(b) = 0\,,$$

Helmholtz equations: $u''(x) + k^2 u(x) = f(x)$, generalized
Helmholtz equations: $u''(x) - k^2 u(x) = f(x)$, Good one!

2D, 3D analogues; practical applications. May or may not be solvable.

$$u''(x) = f(x), \quad a < x < b,$$
$$u'(a) = \alpha, \qquad u(b) = u_b\,.$$

It's wellposed. **Method 1:**

$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f_i, \quad i = 1, 2, \cdots n-1,$$

$$\frac{U_1 - U_0}{h} = \alpha \quad \text{or} \quad \frac{-U_0 + U_1}{h^2} = \frac{\alpha}{h}\,.$$

$$\begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} & & & & \\ \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} & & & \\ & \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} \\ & & & & \frac{1}{h^2} & -\frac{2}{h^2} \end{bmatrix} \begin{bmatrix} U_0 \\ U_1 \\ U_2 \\ \vdots \\ U_{n-2} \\ U_{n-1} \end{bmatrix} = \begin{bmatrix} \frac{\alpha}{h} \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) - \frac{u_b}{h^2} \end{bmatrix}$$

Ghost point method & analysis II

- First order discretization of BC, second order discretization of DE at interior points, expect global error $\|E\|_\infty \sim O(h)$.
- There are n equations, and n unknowns, matched.
- A_h is an M-matrix, invertible.
- Can you prove the convergence?
- What's the local truncation error? $O(h^2)$ interior, $O(1)$ at x_0, why? $u''(x_0) - u'(x_0) = O(1)$!

Ghost point method & analysis III

Idea: Use second order discretization to the Neumann BC.
Method 2: One-sided 2nd order finite difference formula:

$$\frac{-U_2 + 4U_1 - 3U_0}{h} = \alpha$$

Not recommend because (1), the matrix-structure will be changed; (2) hard to prove the stability and convergence.

Method 3: The ghost point method. Extend the soln. to $x_{-1} = x_0 - h$ (outside, ghost point).

- Use ghost point x_{-1} and ghost value U_{-1}. Second order discretization for the DE and BC. Add

$$\frac{U_{-1} - 2U_0 + U_1}{h^2} = f_0, \qquad \frac{U_1 - U_{-1}}{2h} = \alpha,$$

- There are $n+1$ equations, and $n+1$ unknowns, matched.
- Eliminate U_{-1}. $\frac{-2U_0 + \mathbf{2}U_1}{h^2} = f_0 + \frac{2\alpha}{h}$.

The ghost point method II

$$
\begin{bmatrix}
-\frac{2}{h^2} & \frac{2}{h^2} & & & & \\
\frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} & & & \\
& \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} & & \\
& & \ddots & \ddots & \ddots & \\
& & & \frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} \\
& & & & \frac{1}{h^2} & -\frac{2}{h^2}
\end{bmatrix}
\begin{bmatrix}
U_0 \\ U_1 \\ U_2 \\ \vdots \\ U_{n-2} \\ U_{n-1}
\end{bmatrix}
=
\begin{bmatrix}
f_0 + \frac{2\alpha}{h} \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) - \frac{u_b}{h^2}
\end{bmatrix}
$$

- $A_h \in R^{n\times n}$ is an M-matrix. The same structure!
- Second order accurate $\|E\|_\infty \sim O(h^2)$.
- Use the discrete Green function with homogeneous Neumann BC. Project!
- Exercise: Generalize the ghost point method to Robin (mixed) BC and analyze.

The ghost point method III

What's the local truncation error at x_0? Why is it $O(h)$?

$$
\begin{aligned}
T_i &= \frac{-2u(x_i) + 2u(x_1)}{h^2} - \frac{2\alpha h}{h^2} - f_0 \\
&= \frac{u(x_{-1}) - 2u(x_i) + u(x_1) + O(h^3)}{h^2} - f_0 \\
&= O(h) + O(h^2)
\end{aligned}
$$

since $u(x_1) = u(x_{-1}) + 2h\alpha + O(h^3)$.

Rule of thumb: *In general, the local truncation error can be one order lower than that in the interior without affecting global accuracy.*

Conserve FD schemes for 1D self-adjoint S-L problem

$$\left(p(x)u'(x)\right)' - q(x)u(x) = f(x), \quad a < x < b,$$

$$u(a) = u_a, \quad u(b) = u_b, \quad \text{or other BC.}$$

- If $p(x) \in C^1(a,b)$, $q(x) \in C^0(a,b)$, $f(x) \in C^0(a,b)$, $q(x) \geq 0$ and $p(x) \geq p_0 > 0$, then it's wellposed $u(x) \in C^2(a,b)$.
- DO NOT use $pu'' + p'u' - qu = f$, why?
- Use a staggered, (or MAC?) approach! First discretize one derivative at $x_{i+\frac{1}{2}} = x_i + h/2$.

$$\frac{p_{i+\frac{1}{2}} u'(x_{i+\frac{1}{2}}) - p_{i-\frac{1}{2}} u'(x_{i-\frac{1}{2}})}{h} - q_i u(x_i) = f(x_i) + E_i^1,$$

$$\frac{p_{i+\frac{1}{2}} \frac{u(x_{i+1}) - u(x_i)}{h} - p_{i-\frac{1}{2}} \frac{u(x_i) - u(x_{i-1})}{h}}{h} - q_i u(x_i) = f(x_i) + E_i^1 + E_i^2,$$

The matrix-vector form

$$\frac{p_{i+\frac{1}{2}}\, U_{i+1} - \left(p_{i+\frac{1}{2}} + p_{i-\frac{1}{2}}\right) U_i + p_{i-\frac{1}{2}}\, U_{i-1}}{h^2} - q_i U_i = f_i, \tag{6}$$

for $i = 1, 2, \cdots n-1$. In a matrix-vector form, this linear system can be written as $A_h \mathbf{U} = \mathbf{F}$, where

$$A_h = \begin{bmatrix} -\frac{p_{1/2}+p_{3/2}}{h^2} - q_1 & \frac{p_{3/2}}{h^2} & & & \\ \frac{p_{3/2}}{h^2} & -\frac{p_{3/2}+p_{5/2}}{h^2} - q_2 & \frac{p_{5/2}}{h^2} & & \\ & \ddots & \ddots & \ddots & \\ & & & \frac{p_{n-3/2}}{h^2} & -\frac{p_{n-3/2}+p_{n-1/2}}{h^2} - q_{n-1} \end{bmatrix},$$

$$\mathbf{U} = \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \\ U_{n-2} \\ U_{n-1} \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} f(x_1) - \frac{p_{1/2} u_a}{h^2} \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) - \frac{p_{n-1/2} u_b}{h^2} \end{bmatrix}.$$

Conserve FD schemes for 1D self-adjoint S-L problem III

- A_h is still tridiagonal.
- A_h is an M-matrix if the regularity conditions are satisfied.
- The discretization and global solution are both second order accurate! $T_i \sim O(h^2)$, $\|E\|_\infty \sim O(h^2)$.

Not self-adjoint, diffusion and advection equation

- A boundary layer problem:

$$\begin{aligned} \epsilon u'' - u' &= -1, \quad 0 < x < 1, \\ u(0) = 1, & \qquad u(1) = 3. \end{aligned}$$

- More general form

$$\begin{aligned} & \left(p(x)u'(x)\right)' + b(x)u'(x) - q(x)u(x) = f(x), \quad a < x < b, \\ & u(a) = u_a, \quad u(b) = u_b, \quad \text{or other BC.} \end{aligned}$$

- Central schemes if the advection is small $b| \leq \frac{C}{h}$.
- Upwinding, first order
- Integrating factor + scaling $\Longrightarrow$ Change the problem to a self-adjoint? How?

Integrating factor + scaling strategy

- Idea: multiplying an integrating factor to eliminate the advection term.

$$\mu \left\{ \left(pu'\right)' + bu' - qu \right\} = \mu f$$

$$\Longrightarrow \left(\mu p u'\right)' - \mu' p u' + \mu b u' - q \mu u = \mu f$$

$$\Longrightarrow \mu(x) = \int e^{b(x)/p(x)} dx$$

- New ODE is a diffusion equation. Integral operation is a good operator. Let $\bar{p}$ be the average of p in $(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$.

$$\left(\mu p u'\right)' - q\mu u = \mu f, \qquad \text{scaling}$$

$$\frac{1}{\bar{p}} \left\{ \frac{p_{i+\frac{1}{2}} U_{i+1} - \left(p_{i+\frac{1}{2}} + p_{i-\frac{1}{2}}\right) U_i + p_{i-\frac{1}{2}} U_{i-1}}{h^2} - q_i U_i = f_i \right\}$$

Validation and data analysis

- Use known exact solution and check how the error changes called grid refinement analysis

$$n = 40, \quad \|E_{40}\|, \quad n = 80, \quad \|E_{80}\|, \quad \frac{\|E_{40}\|}{\|E_{80}\|}, \quad \cdots,$$

$$\text{ratios} \quad \frac{\|E_N\|}{\|E_{2N}\|}, \qquad \text{rate} \quad p = \frac{\left|\log \frac{\|E_N\|}{\|E_{2N}\|}\right|}{\log 2}$$

- How to choose exact solutions? Set u first, find f and BCs, called manufactoried solution. Not always easy!
- First order method, ratio ≈ 1, oder ≈ 1; Second order method, ratio ≈ 4, oder ≈ 2.

Validation and data analysis II

- If problem is too complicated, then we can use the solution obtained from a finest grid, say, $n = 1024$, but the ratios and rates will be different.
- Wrongly used in the literature, discovered by Zhilin Li

$$u_h = u_e + Ch^p + \cdots$$

$$u_{h_*} = u_e + C{h_*}^p + \cdots$$

$$u_h - u_{h_*} \approx C\left(h^p - {h_*}^p\right),$$

$$u_{h/2} - u_{h_*} \approx C\left((h/2)^p - {h_*}^p\right)$$

$$\frac{\tilde{u}(h) - \tilde{u}(h^*)}{\tilde{u}(\frac{h}{2}) - \tilde{u}(h^*)} = \frac{2^p\left(1 - 2^{-kp}\right)}{1 - 2^{p(1-k)}}$$

$$3, \quad \frac{7}{3} \simeq 2.333, \quad \frac{15}{7} \simeq 2.1429, \quad \frac{31}{15} \simeq 2.067, \quad \cdots.$$

$$5, \quad \frac{63}{15} = 4.2, \quad \frac{255}{63} \simeq 4.0476, \quad \frac{1023}{255} \simeq 4.0118, \quad \cdots$$

A fourth order compact scheme for 1D Poisson equation

$$u''(x) = f(x), \quad a < x < b,$$

$$u(a) = \alpha, \qquad u(b) = u_b \,.$$

- It's possible to use a 5-point stencil 4th order scheme, not recommended, why?
  Not compact, doest not work near BC, matrix structure changed (not an M-matrix), hard to discuss the stability.
- Use finite difference operator to derive high order compact schemes.

$$\begin{aligned}
\delta_{xx}^2 u &= \frac{d^2 u}{dx^2} + \frac{h^2}{12}\frac{d^4 u}{dx^4} + O(h^4) \\
&= \left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right)\frac{d^2}{dx^2}\, u + O(h^4) \\
&= \left(1 + \frac{h^2}{12}\delta_{xx}^2\right)\frac{d^2}{dx^2}\, u + O(h^4)\,,
\end{aligned}$$

A fourth order compact scheme for 1D Poisson equation

Solve for $\frac{d^2u}{dx^2}$

$$\frac{d^2}{dx^2}\,u = \left(1 + \frac{h^2}{12}\delta_{xx}^2\right)^{-1}\delta_{xx}^2 u + O(h^4)$$

The fourth order compact scheme is

$$\left(1 + \frac{h^2}{12}\delta_{xx}^2\right)^{-1}\delta_{xx}^2 U_i = f_i$$

$$\delta_{xx}^2 U_i = \left(1 + \frac{h^2}{12}\delta_{xx}^2\right) f_i$$

$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f(x_i) + \frac{1}{12}\left(f_{i-1} - 2f_i + f_{i+1}\right)$$

Motivations (smaller matrices, oscillatory solutions), other methods, Richardson extrapolation.