Finite difference approximation

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Finite difference method (FDM)

Consider an ODE

$$-au'' + bu' + cu = 0 \qquad x \in (0,1)$$

with some boundary conditions.

Basic idea of finite difference method: Discretize the domain $\Omega = (0,1)$ with N points known as *grid* or *mesh*

$$0 = x_1 < \ldots < x_{N-1} < x_N = 1$$

Usually

$$x_{j+1} - x_j = h = \Delta x$$

Approximate derivatives with finite differences

$$Du_j \approx u'(x_j) \qquad\qquad D^2u_j \approx u''(x_j)$$

Satisfy the ODE at the grid points in an approximate sense: $U_j \approx u(x_j)$

$$-a_j D^2 U_j + b_j D U_j + c_j U_j = 0 \qquad 2 \le j \le N-1$$

Somehow solve for the unknown values $U_2, U_3, \ldots, U_{N-1}$.

Finite difference approximation

Derivatives as limits (we take $h > 0$ always)

$$u'(x_j) = \lim_{h\to 0} \frac{u(x_j + h) - u(x_j)}{h} = \lim_{h\to 0} \frac{u(x_j) - u(x_j - h)}{h}$$

Finite difference approximation: Take finite h; many possibilities

$$\text{Forward difference (FD)}: \qquad D_x^+ u_j = \frac{u_{j+1} - u_j}{h}$$

$$\text{Backward difference (BD)}: \qquad D_x^- u_j = \frac{u_j - u_{j-1}}{h}$$

$$\text{Central difference (CD)}: \qquad D_x^0 u_j = \frac{u_{j+1} - u_{j-1}}{2h}$$

Since they were obtained from the definition of the derivative, they must provide consistent approximation of the derivative.

Consistency of forward difference $D_x^+ u_j$

Taylor formula around $x = x_j$

$$u_{j+1} = u_j + h u_j' + \frac{h^2}{2} u_j'' + \mathcal{O}\left(h^3\right)$$

$$\frac{u_{j+1} - u_j}{h} = u_j' + \frac{h}{2} u_j'' + \mathcal{O}\left(h^2\right)$$

Error

$$D_x^+ u_j - u_j' = \frac{h}{2} u_j'' + \mathcal{O}\left(h^2\right)$$

Or, use Taylor formula with remainder term

$$D_x^+ u_j - u_j' = \frac{h}{2} u''(\xi), \qquad \xi \in [x_j, x_{j+1}]$$

Typical error estimate

$$|D_x^+ u_j - u_j'| \le \frac{1}{2} h \sup_x |u''(x)| = \mathcal{O}\left(h\right)$$

If $u \in \mathcal{C}^2(0,1)$: D_x^+ is consistent and first order accurate

Consistency of backward difference D_x^-

Taylor formula around $x = x_j$

$$u_{j-1} = u_j - hu_j' + \frac{h^2}{2}u_j'' + \mathcal{O}\left(h^3\right)$$

$$\frac{u_j - u_{j-1}}{h} = u_j' + \frac{h}{2}u_j'' + \mathcal{O}\left(h^2\right)$$

Error

$$D_x^- u_j - u_j' = \frac{h}{2}u_j'' + \mathcal{O}\left(h^2\right)$$

Or, use Taylor formula with remainder term

$$D_x^- u_j - u_j' = \frac{h}{2}u''(\xi), \qquad \xi \in [x_j, x_{j+1}]$$

Typical error estimate

$$|D_x^- u_j - u_j'| \le \frac{1}{2}h \sup_x |u''(x)| = \mathcal{O}\left(h\right)$$

If $u \in \mathcal{C}^2(0,1)$: D_x^- is consistent and first order accurate

Consistency of central difference D_x^0

Taylor formula around $x = x_j$

$$u_{j+1} = u_j + hu'_j + \frac{h^2}{2}u''_j + \frac{h^3}{6}u'''_j + \mathcal{O}\left(h^4\right)$$

$$u_{j-1} = u_j - hu'_j + \frac{h^2}{2}u''_j - \frac{h^3}{6}u'''_j + \mathcal{O}\left(h^4\right)$$

$$\frac{u_{j+1} - u_{j-1}}{2h} = u'_j + \frac{h^2}{6}u'''_j + \mathcal{O}\left(h^4\right)$$

Error

$$D_x^0 u_j - u'_j = \frac{h^2}{6}u''_j + \mathcal{O}\left(h^3\right)$$

Or, using Taylor formula with remainder term

$$|D_x^0 u_j - u'_j| \le \frac{1}{3}h^2 \sup_x |u'''(x)| = \mathcal{O}\left(h^2\right)$$

If $u \in \mathcal{C}^3(0,1)$: D_x^0 is consistent and second order accurate

Consistency of central difference when $u \notin \mathcal{C}^3(0,1)$

What if $u \in \mathcal{C}^2(0,1)$ but $u \notin \mathcal{C}^3(0,1)$

$$u_{j+1} = u_j + hu'_j + \frac{h^2}{2}u''(\xi), \qquad \xi \in [x_j, x_{j+1}]$$

$$u_{j-1} = u_j - hu'_j + \frac{h^2}{2}u''(\eta), \qquad \eta \in [x_{j-1}, x_j]$$

$$\frac{u_{j+1} - u_{j-1}}{2h} = u'_j + \frac{h}{4}[u''(\xi) - u''(\eta)]$$

Error

$$D_x^0 u_j - u'_j = \frac{h}{4}[u''(\xi) - u''(\eta)]$$

Or

$$|D_x^0 u_j - u'_j| \le \frac{1}{2} h \sup_x |u''(x)| = \mathcal{O}(h)$$

If $u \in \mathcal{C}^2(0,1)$: D_x^0 is consistent and first order accurate

Generation of FD formulae

Suppose we want to approximate

$$u'(x_j) \qquad \text{using} \qquad u_{j-2}, u_{j-1}, u_j$$

Assume a formula with unknown coefficients a, b, c

$$Du_j = a u_{j-2} + b u_{j-1} + c u_j \approx u'_j, \qquad \text{(non-centered)}$$

Use Taylor formula around $x = x_j$

$$\begin{aligned} Du_j &= a\left[u_j - 2hu'_j + 2h^2 u''_j - \frac{4}{3}h^3 u'''_j + \mathcal{O}\left(h^4\right)\right] \\ &\quad + b\left[u_j - hu'_j + \frac{1}{2}h^2 u''_j - \frac{1}{6}h^3 u'''_j + \mathcal{O}\left(h^4\right)\right] \\ &\quad + c u_j \\ &= (a+b+c)u_j - (2a+b)hu'_j + (2a + \frac{1}{2}b)h^2 u''_j \\ &\quad - (\frac{4}{3}a + \frac{1}{6}b)h^3 u'''_j + \mathcal{O}\left(h^3\right) \end{aligned}$$

Generation of FD formulae

Choose a, b, c so that

$$\begin{aligned} a + b + c &= 0 \\ -(2a + b)h &= 1 \\ 2a + \frac{1}{2}b &= 0 \end{aligned}$$

Unique solution is

$$a = \frac{1}{2h}, \qquad b = -\frac{2}{h}, \qquad c = \frac{3}{2h}$$

Hence the FD formula is

$$Du_j = \frac{u_{j-2} - 4u_{j-1} + 3u_j}{2h}$$

Error estimate

$$Du_j - u_j' = -(\frac{4}{3}a + \frac{1}{6}b)h^3 u_j''' + \mathcal{O}\left(h^3\right) = -\frac{1}{3}h^2 u_j''' + \mathcal{O}\left(h^3\right)$$

If $u \in \mathcal{C}^3(0,1)$: Consistent and second order accurate

Some remarks

- Approximate $u'(x_j)$ using $u_{j-2}, u_{j-1}, u_j, u_{j+1}, u_{j+2}$

$$Du_j = \frac{1}{2h}(u_{j-2} - 8u_{j-1} + 8u_{j+1} - u_{j+2}) = u'(x_j) + \mathcal{O}\left(h^4\right)$$

  - central difference approximation
  - Note the *anti-symmetric* structure of the formula
- To obtain higher order accuracy, we need to increase the stencil size
- Higher order accuracy requires higher regularity/smoothness of the function
- Central difference formulae give more accuracy with <u>compact stencil</u> as compared to one-sided or non-centered stencil

Differentiation via interpolation

Construct approximation to $u'(x_j)$ using

$$\{u_{j-k}, \dots, u_{j-1}, u_j, u_{j+1}, \dots, u_{j+l}\} \qquad k+l+1 \text{ points}$$

Write an interpolating polynomial

$$p_j(x) = \sum_{r=j-k}^{j+l} L_r(x) u_r, \qquad L_r(x_s) = \delta_{rs}$$

$$L_r(x) = \frac{(x - x_{j-k}) \dots (x - x_{r-1})(x - x_{r+1}) \dots (x - x_{j+l})}{(x_r - x_{j-k}) \dots (x_r - x_{r-1})(x_r - x_{r+1}) \dots (x_r - x_{j+l})}$$

Approximation of derivative

$$u'(x_j) \approx p_j'(x_j) = \sum_{r=j-k}^{j+l} L_r'(x_j) u_r$$

Can be used on non-uniform grids also.

Approximation of second derivative

$$u''(x_j) = \lim_{h \to 0} \frac{u'(x_j + h/2) - u'(x_j - h/2)}{h}$$

Finite difference

$$u''(x_j) \approx \frac{u'(x_j + h/2) - u'(x_j - h/2)}{h} \approx \frac{\frac{u_{j+1} - u_j}{h} - \frac{u_j - u_{j-1}}{h}}{h}$$

$$D^2 u_j = \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} = u''(x_j) + \mathcal{O}\left(h^2\right)$$

- Note the *symmetric* structure of the formula
- Other methods
  - Generate formulae by matching Taylor series
  - Or, use the method of interpolating polynomial

Non-uniform grids

Non-uniform grids essential to capture rapid variations, e.g., boundary layers

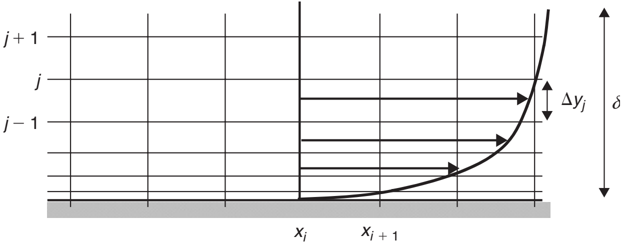
$$x_1 < x_2 < \ldots < x_N, \qquad x_{j+1} - x_j = h_j \neq \text{constant}$$

Finite difference

$$\frac{u_j - u_{j-1}}{x_j - x_{j-1}} = u'(x_j) + \mathcal{O}\left(x_j - x_{j-1}\right), \qquad \frac{u_{j+1} - u_j}{x_{j+1} - x_j} = u'(x_j) + \mathcal{O}\left(x_{j+1} - x_j\right)$$

$$\frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}} = u'(x_j) + \mathcal{O}\left(x_{j+1} - x_{j-1}\right)$$

In general, all of these are first order accurate. Central difference does not give high accuracy as in case of uniform grids.



Smooth non-uniform grids

<u>Example</u>: Suppose $x \in [0, 1]$. Do a change of variable, e.g.,

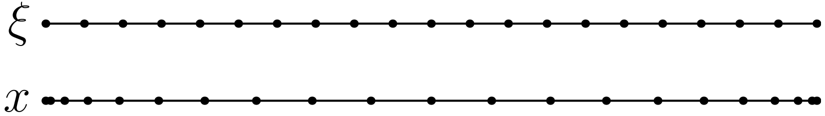
$$x = f(\xi) = \frac{1}{2}[1 - \cos(\pi\xi)], \qquad \xi \in [0, 1]$$

Make a *uniform grid* in ξ-space, also called ***computational space***

$$\xi_1 < \xi_2 < \ldots < \xi_N, \qquad \xi_j - \xi_{j-1} = \Delta\xi = \frac{1}{N-1}$$

Associated grid in ***physical space***

$$x_j = f(\xi_j), \qquad 1 \le j \le N$$



$$\frac{\mathrm{d}u}{\mathrm{d}x} = \frac{\mathrm{d}u}{\mathrm{d}\xi}\frac{\mathrm{d}\xi}{\mathrm{d}x}$$

Finite difference approximation

$$\frac{\mathrm{d}u}{\mathrm{d}x}(x_j) \approx \frac{u_{j+1} - u_{j-1}}{2\Delta\xi}\frac{\mathrm{d}\xi}{\mathrm{d}x}(x_j)$$

Spectral analysis

$f : [0,1] \to \mathbb{R}$ a periodic function. Discrete Fourier series approximation

$$f = \sum_{k=-N/2}^{N/2} \hat{f}_k \mathrm{e}^{\mathrm{i}2\pi kx}, \qquad \hat{f}_{-k} = \hat{f}_k^*$$

How does the finite difference approximate derivatives of Fourier modes

$$f(x) = \mathrm{e}^{\mathrm{i}2\pi kx}, \qquad 0 \le k \le N/2$$

Exact derivative

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x_j) = \mathrm{i}2\pi k \mathrm{e}^{\mathrm{i}2\pi kx_j}$$

Central difference

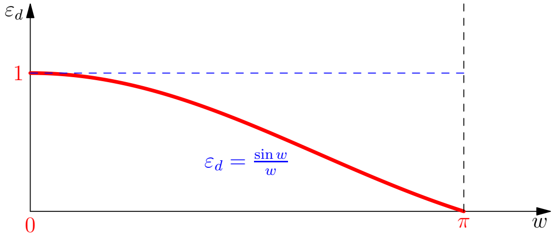
$$D_x^0 f_j = \frac{f_{j+1} - f_{j-1}}{2h} = \frac{\mathrm{e}^{\mathrm{i}2\pi k(x_j+h)} - \mathrm{e}^{\mathrm{i}2\pi k(x_j-h)}}{2h} = \mathrm{i}\frac{\sin(2\pi kh)}{h}\mathrm{e}^{\mathrm{i}2\pi kx_j}$$

$$D_x^0 f_j = \frac{\sin(2\pi kh)}{2\pi kh}\mathrm{i}2\pi k\mathrm{e}^{\mathrm{i}2\pi kx_j} = \frac{\sin(2\pi kh)}{2\pi kh}\frac{\mathrm{d}f}{\mathrm{d}x}(x_j)$$

Spectral analysis

Ratio of numerical to exact amplitude (Note: $h = 1/N$)

$$w = 2\pi k h, \qquad \varepsilon_d = \frac{\sin(2\pi k h)}{2\pi k h} = \frac{\sin(w)}{w} = \frac{w'(w)}{w}, \qquad 0 \le w \le \pi$$



- Central finite difference is able to resolve only small wavenumbers k, i.e., $w \ll \pi$, i.e., very smooth functions
- For large k, i.e., $w \approx \pi$, the functions are rapidly varying. Finite difference damps these high frequency modes excessively.
- Desirable to have $\varepsilon_d \approx 1$ over a larger range of w
  Very important for convection problems

Compact schemes (Lele)

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_i + \alpha f'_{i+1} + \beta f'_{i+2}$$
$$= c\,\frac{f_{i+3} - f_{i-3}}{6h} + b\,\frac{f_{i+2} - f_{i-2}}{4h} + a\,\frac{f_{i+1} - f_{i-1}}{2h}.$$

Match terms in Taylor series about x_i on both sides

$$a + b + c = 1 + 2\alpha + 2\beta \qquad \text{(second order)} \qquad (2.1.1)$$

$$a + 2^2 b + 3^2 c = 2\,\frac{3!}{2!}(\alpha + 2^2\beta) \qquad \text{(fourth order)} \qquad (2.1.2)$$

$$a + 2^4 b + 3^4 c = 2\,\frac{5!}{4!}(\alpha + 2^4\beta) \qquad \text{(sixth order)} \qquad (2.1.3)$$

$$a + 2^6 b + 3^6 c = 2\,\frac{7!}{6!}(\alpha + 2^6\beta) \qquad \text{(eighth order)} \qquad (2.1.4)$$

$$a + 2^8 b + 3^8 c = 2\,\frac{9!}{8!}(\alpha + 2^8\beta) \qquad \text{(tenth order).} \qquad (2.1.5)$$

Compact schemes (Lele)

Example: Three point stencil, $\beta = b = c = 0$

$$\alpha f'_{i-1} + f'_i + \alpha f'_{i+1} = a \frac{f_{i+1} - f_{i-1}}{2h}$$

Two unknowns a, α, we need two equations 2.1.1 and 2.1.2

$$a = 1 + 2\alpha, \qquad a = 2\frac{3!}{2!}\alpha = 6\alpha \quad \Longrightarrow \quad a = \frac{3}{2}, \quad \alpha = \frac{1}{4}$$

- Need some boundary condition: periodic or one-sided formulae
- Stencil is $\{i-1, i, i+1\}$
- Implicit; solve for $\{f'_i\}$ by solving tri-diagonal matrix problem
  Can be done very efficiently using Thomas Tridiagonal Algorithm
- The approximation is fourth order accurate.
- Classical Pade scheme

Compact schemes (Lele)

Tridiagonal schemes: $\beta = 0$

Fourth order, one parameter α

$$\beta = 0, \quad a = \tfrac{2}{3}(\alpha + 2), \quad b = \tfrac{1}{3}(4\alpha - 1), \quad c = 0. \qquad (2.1.6)$$

Sixth order

$$\alpha = \tfrac{1}{3}, \quad \beta = 0, \quad a = \tfrac{14}{9}, \quad b = \tfrac{1}{9}, \quad c = 0. \qquad (2.1.7)$$

Sixth order, one parameter α

$$\begin{gathered} \beta = 0, \quad a = \tfrac{1}{6}(\alpha + 9), \\ b = \tfrac{1}{15}(32\alpha - 9), \quad c = \tfrac{1}{10}(-3\alpha + 1). \end{gathered} \qquad (2.1.8)$$

Compact schemes (Lele)

Truncation Error for the First Derivative Schemes

Scheme	Max. l.h.s. stencil size	Max. r.h.s. stencil size	Truncation error in (2.1)
(2.1.6)	3	5	$\frac{4}{5!}(3\alpha-1)h^4f^{(5)}$
(2.1.7)	3	5	$\frac{4}{7!}h^6f^{(7)}$
(2.1.8)	3	7	$\frac{12}{7!}(-8\alpha+3)h^6f^{(7)}$
(2.1.8) & $\alpha=\frac{3}{8}$	3	7	$\frac{-36}{9!}h^8f^{(9)}$
(2.1.9)	5	7	$\frac{4}{5}(-1+3\alpha-12\beta+10c)h^4f^{(5)}$
(2.1.10)	5	7	$\frac{12}{7!}(3-8\alpha+20\beta)h^6f^{(7)}$
(2.1.11)	5	5	$\frac{4}{7!}(9\alpha-4)h^6f^{(7)}$
(2.1.12)	5	5	$-\frac{16}{9!}h^8f^{(9)}$
(2.1.13)	5	7	$\frac{144}{9!}(2\alpha-1)h^8f^{(9)}$
(2.1.14)	5	7	$\frac{144}{11!}h^{10}f^{(11)}$

Compact schemes: Spectral analysis

$$w'(w) = \frac{a\sin(w) + (b/2)\sin(2w) + (c/3)\sin(3w)}{1 + 2\alpha\cos(w) + 2\beta\cos(2w)}. \qquad (3.1.4)$$

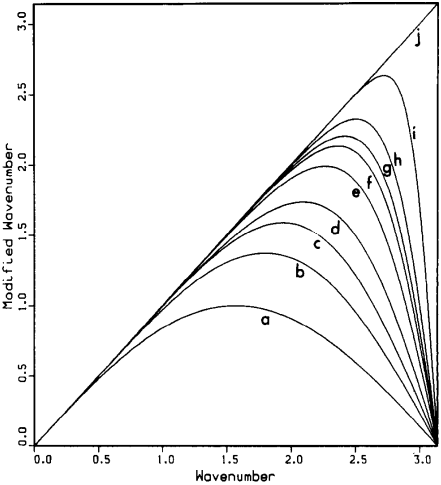


FIG. 1. Plot of modified wavenumber vs wavenumber for first derivative approximations: (a) second-order central differences; (b) fourth-order central differences; (c) sixth-order central differences; (d) standard Padé scheme ($\beta = 0 = c$, $\alpha = \frac{1}{4}$); (e) sixth-order tridiagonal scheme ($\beta = 0 = c$, $\alpha = \frac{1}{3}$); (f) eighth-order tridiagonal scheme ($\beta = 0$); (g) eighth-order pentadiagonal scheme ($c = 0$); (h) tenth-order pentadiagonal scheme; (i) spectral-like pentadiagonal scheme (3.1.6); (j) exact differentiation.