Compact Finite Difference Schemes

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Math 228B Numerical Solutions of Differential Equations

Approximation of First Derivative

- Consider a uniformly spaced mesh $x_i = hi$ with given function values $f_i = f(x_i)$. Seek approximations to the first derivative at the nodes $f_i' = f'(x_i)$ of the form

$$\begin{aligned}\beta f_{i-2}' + \alpha f_{i-1}' + f_i' + \alpha f_{i+1}' + \beta f_{i+2}' \\ = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}\end{aligned}$$

- Match Taylor series coefficients for order conditions:

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

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

$$a + 2^4 b + 3^4 c = 2\frac{5!}{4!}(\alpha + 2^4\beta) \qquad \text{(6th order)}$$

$$a + 2^6 b + 3^6 c = 2\frac{7!}{6!}(\alpha + 2^6\beta) \qquad \text{(8th order)}$$

$$a + 2^8 b + 3^8 c = 2\frac{9!}{8!}(\alpha + 2^8\beta) \qquad \text{(10th order)}$$

Tridiagonal Schemes

- If $\beta = 0$ and α nonzero, tridiagonal systems need to be solved to obtain the derivative approximations
- If in addition $c = 0$, a one-parameter (α) family of 4th order tridiagonal schemes is obtained:

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

- Special cases:
  - $\alpha = 0$ gives the standard 4th order central difference scheme,
  - $\alpha = 1/4$ gives the classical Padé scheme.
  - $\alpha = 1/3$ gives a 6th order accurate scheme:

$$\alpha = \frac{1}{3}, \quad \beta = 0, \quad a = \frac{14}{9}, \quad b = \frac{1}{9} \quad c = 0$$

Tridiagonal Schemes

- If $\beta = 0$ and $c \neq 0$, a one-parameter (α) family of 6th order tridiagonal schemes is obtained:

$$\beta = 0, \quad a = \frac{1}{6}(\alpha + 9), \quad b = \frac{1}{15}(32\alpha - 9), \quad c = \frac{1}{10}(-3\alpha + 1)$$

- Special cases:
  - $\alpha = 3/8$ gives an 8th order accurate scheme:

$$\beta = 0, \quad a = \frac{25}{16}, \quad b = \frac{1}{5}, \quad c = -\frac{1}{80}$$

Pendadiagonal Schemes

- If $\beta \neq 0$ and $c = 0$, a one-parameter (α) family of 6th order pentadiagonal schemes is obtained:

$$\beta = \frac{1}{12}(-1 + 3\alpha), \quad a = \frac{2}{9}(8 - 3\alpha), \quad b = \frac{1}{18}(-17 + 57\alpha), \quad c = 0$$

which becomes an 8th order scheme if $\alpha = 4/9$:

$$\alpha = \frac{4}{9}, \quad \beta = \frac{1}{36}, \quad a = \frac{40}{27}, \quad b = \frac{25}{54}, \quad c = 0$$

- If $\beta \neq 0$ and $c \neq 0$, a one-parameter (α) family of 8th order pentadiagonal schemes is obtained:

$$\beta = \frac{1}{20}(-3 + 8\alpha), \; a = \frac{1}{6}(12 - 7\alpha), \; b = \frac{1}{150}(568\alpha - 183), \; c = \frac{1}{50}(9\alpha - 4)$$

which becomes a 10th order scheme if $\alpha = 1/2$:

$$\alpha = \frac{1}{2}, \quad \beta = \frac{1}{20}, \quad a = \frac{17}{12}, \quad b = \frac{101}{150}, \quad c = \frac{1}{100}$$

Approximation of Second Derivative

- Seek approximations to the second derivative at the nodes $f_i'' = f''(x_i)$ of the form

$$\beta f_{i-2}'' + \alpha f_{i-1}'' + f_i'' + \alpha f_{i+1}'' + \beta f_{i+2}''$$
$$= c\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

- Match Taylor series coefficients for order conditions:

$$a + b + c = 1 + 2\alpha + 2\beta \qquad \text{(2nd order)}$$
$$a + 2^2 b + 3^2 c = 2\frac{4!}{2!}(\alpha + 2^2\beta) \qquad \text{(4th order)}$$
$$a + 2^4 b + 3^4 c = 2\frac{6!}{4!}(\alpha + 2^4\beta) \qquad \text{(6th order)}$$
$$a + 2^6 b + 3^6 c = 2\frac{8!}{6!}(\alpha + 2^6\beta) \qquad \text{(8th order)}$$
$$a + 2^8 b + 3^8 c = 2\frac{10!}{8!}(\alpha + 2^8\beta) \qquad \text{(10th order)}$$

Tridiagonal Schemes

- If $\beta = 0$ and $c = 0$, a one-parameter (α) family of 4th order tridiagonal schemes is obtained:

$$\beta = 0, \quad c = 0, \quad a = \frac{4}{3}(1-\alpha), \quad b = \frac{1}{3}(-1+10\alpha)$$

- Special cases:
  - $\alpha = 0$ gives the standard 4th order central difference scheme,
  - $\alpha = 1/10$ gives the classical Padé scheme.
  - $\alpha = 2/11$ gives a 6th order accurate scheme:

$$\alpha = \frac{2}{11}, \quad \beta = 0, \quad a = \frac{12}{11}, \quad b = \frac{3}{11}, \quad c = 0$$

- Similarly to before, higher order and pentadiagonal schemes can be derived

Fourier Analysis

- Assume periodic domain $[0, L]$ with $f_1 = f_{N+1}$ and $h = L/N$
- Decompose variables into fourier coefficients

$$f(x) = \sum_{k=-N/2}^{n=N/2} \hat{f}_k \exp\left(\frac{2\pi ikx}{L}\right)$$

- Introduced scaled wavenumber $w = 2\pi kh/L = 2\pi k/N$ in the domain $[0, \pi]$, and the scaled coordinate $s = x/h$, giving Fourier modes $\exp(iws)$
- The exact first derivative generates Fourier coefficients $\hat{f}'_k = iw\hat{f}_k$
- Compare with the coefficients $(\hat{f}'_k)_{fd} = iw'\hat{f}_k$ obtained from the differencing scheme

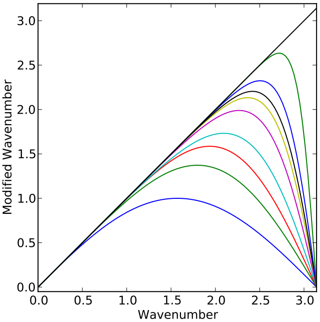
Modified wavenumber, first derivatives

- The first derivative approximations:

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

corresponds to

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



From bottom to top: 2nd order central, 4th order central, 4th order central, standard Padé, 6th order tridiagonal, 8th order tridiagonal, 8th order pentadiagonal, 10th order pentadiagonal, spectral-like, exact differentiation

Modified wavenumber, second derivatives

- The exact second derivative generates Fourier coefficients $\hat{f}''_k = -w^2 \hat{f}_k$
- Compare with the coefficients $(\hat{f}''_k)_{fd} = -w'' \hat{f}_k$ obtained from the differencing scheme
- The second derivative approximations:

$$\beta f''_{i-2} + \alpha f''_{i-1} + f''_i + \alpha f''_{i+1} + \beta f''_{i+2}$$
$$= c\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

corresponds to

$$w''(w) = \frac{2a(1 - \cos(w)) + (b/2)(1 - \cos(2w)) + (2c/9)(1 - \cos(3w))}{1 + 2\alpha \cos(w) + 2\beta \cos(2w)}$$

Non-Periodic Boundaries

- Find first derivative at the boundary $i = 1$ by one-sided approximation:

$$f'_1 + \alpha f'_2 = \frac{1}{h}(af_1 + bf_2 + cf_3 + df_4)$$

- 2nd order accuracy requires

$$a = -\frac{3 + \alpha + 2d}{2}, \quad b = 2 + 3d, \quad c = -\frac{1 - \alpha + 6d}{2}$$

- Third and fourth order schemes can also be derived
- Harder to study using Fourier analysis

Filtering

- Find filtered values $\hat{f}_i$ from an approximation

  $$\beta\hat{f}_{i-2} + \alpha\hat{f}_{i-1} + \hat{f}_i + \alpha\hat{f}_{i+1} + \beta\hat{f}_{i+2}$$
  $$= a f_i + \frac{d}{2}(f_{i+3} + f_{i-3}) + \frac{c}{2}(f_{i+2} + f_{i-2}) + \frac{b}{2}(f_{i+1} + f_{i-1})$$

  with transfer function

  $$T(w) = \frac{a + b\cos(w) + c\cos(2w) + d\cos(3w)}{1 + 2\alpha\cos(w) + 2\beta\cos(2w)}$$

- Impose $T(\pi) = 0$, and possibly higher order derivatives
- Match Taylor series coefficients for high formal accuracy

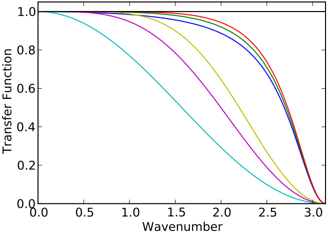
Filtering

- Set $\beta = 0$ for tridiagonal system, use one free parameter $-0.5 < \alpha \leq 0.5$:

$$(F2) \quad a = \frac{1}{2} + \alpha, \quad b = \frac{1}{2} + \alpha$$

$$(F4) \quad a = \frac{5}{8} + \frac{3\alpha}{4}, \quad b = \frac{1}{2} + \alpha \quad c = -\frac{1}{8} + \frac{\alpha}{4}$$

$$(F6) \quad a = \frac{11}{16} + \frac{5\alpha}{8}, \quad b = \frac{15}{32} + \frac{17\alpha}{16}, \quad c = -\frac{3}{16} + \frac{3\alpha}{8}, \quad d = \frac{1}{32} - \frac{\alpha}{16}$$



From left to right:
$(F2)$ $\alpha = 0$, $(F4)$ $\alpha = 0$, $(F6)$ $\alpha = 0$,
$(F2)$ $\alpha = 0.45$, $(F4)$ $\alpha = 0.45$,
$(F6)$ $\alpha = 0.45$,