Higher-Order Finite Difference Scheme for Spatial Derivatives

Fu and Hu (1995) show a procedure on how to obtain the higher order $f^{(k)}(x_0) = f_0^{(k)}$ in a simulation system with uniform grid distribution.

Let the grid size be h, and let $f_0^{(k)} = \frac{1}{h^k}(\sum_{l=-n}^{+n} a_l f_l) + R$.

The Taylor expansion with respect to $x = x_0$ yields

$$a_0(f_0 = f_0)$$

$$a_{\pm 1}[f_{\pm 1} = f_0 \pm h f_0' + \frac{h^2}{2} f_0'' \pm \frac{h^3}{6} f_0^{(3)} + \frac{h^4}{24} f_0^{(4)} \pm \frac{h^5}{120} f_0^{(5)}$$

$$+ \frac{h^6}{720} f_0^{(6)} \pm \frac{h^7}{5040} f_0^{(7)} + O(h^8 f_0^{(8)})]$$

$$a_{\pm 2}[f_{\pm 2} = f_0 \pm (2h)f_0' + \frac{(2h)^2}{2} f_0'' \pm \frac{(2h)^3}{6} f_0^{(3)} + \frac{(2h)^4}{24} f_0^{(4)} \pm \frac{(2h)^5}{120} f_0^{(5)} + \frac{(2h)^6}{720} f_0^{(6)} \pm \frac{(2h)^7}{5040} f_0^{(7)} + O(h^8 f_0^{(8)})]$$

and so on. Thus

$$\sum_{l=-n}^{n} a_l f_l = [a_0 + (a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) + (a_{+3} + a_{-3}) + \ldots + (a_{+n} + a_{-n})] f_0$$

$$+ [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2 + (a_{+3} + a_{-3}) \cdot 3 + \ldots + (a_{+n} + a_{-n}) \cdot n] f_0' \cdot h$$

$$+ [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^2 + (a_{+3} + a_{-3}) \cdot 3^2 + \ldots + (a_{+n} + a_{-n}) \cdot n^2] f_0'' \cdot \frac{h^2}{2}$$

$$+ [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^3 + (a_{+3} + a_{-3}) \cdot 3^3 + \ldots + (a_{+n} + a_{-n}) \cdot n^3] f_0^{(3)} \cdot \frac{h^3}{3!}$$

$$+ \ldots \tag{1}$$

Substituting equation (1) into $f_0^{(k)} = \frac{1}{h^k}(\sum_{l=-n}^{+n} a_l f_l) + R$ and comparing the coefficients, it yields

$$[(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^k + (a_{+3} + a_{-3}) \cdot 3^k + \ldots + (a_{+n} + a_{-n}) \cdot n^k] = k! \tag{2}$$

and

$$[(a_{+1}+a_{-1})+(a_{+2}+a_{-2})\cdot 2^{j}+(a_{+3}+a_{-3})\cdot 3^{j}+\ldots+(a_{+n}+a_{-n})\cdot n^{j}]=0 \qquad (3)$$

for $j=0\to n$, but $j\neq k$.

The coefficients $a_{\pm l}$ of the finite difference expression of $f_0^{(k)}$ can be obtained by solving above system equations (2) and (3)

Determine $f^{(k)}(x)$ *for an even number* k

Let $a_l - a_{-l} = 0$ and $b_l = a_l + a_{-l} = 2a_l$. It yields $a_0 = -(b_1 + b_2 + ... + b_n)$ and $b_1, b_2, b_3, ..., b_n$ satisfy

$$[b_1 + b_2 \cdot 2^k + b_3 \cdot 3^k + ... + b_n \cdot n^k] = k! \tag{4}$$

$$[b_1 + b_2 \cdot 2^j + b_3 \cdot 3^j + ... + b_n \cdot n^j] = 0 \tag{5}$$

where j is an even number and $j \neq k$. Eqs. (4) and (5) can be rewritten as

$$\begin{bmatrix} 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ 1 & 2^4 & 3^4 & \cdots & \cdots & n^4 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ k! \\ 0 \\ \vdots \end{bmatrix} \tag{6}$$

The matrix on the left-hand side of Eq. (6) is called the Vandermonde matrix.

In summary, for an *even number* k

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ 1 & 2^4 & 3^4 & \cdots & \cdots & n^4 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ k! \\ 0 \\ \vdots \end{bmatrix} \qquad (7)$$

$a_l = a_{-l}$, $a_0 = -2(a_1 + a_2 + \ldots + a_n)$, and

$$f_0^{(k)} = \frac{1}{h^k}[\sum_{l=-n}^{+n} a_l f_l + O(h^{2n+2} f_0^{(2n+2)})] = \frac{1}{h^k}(\sum_{l=-n}^{+n} a_l f_l) + O(h^{2n+2-k} f_0^{(2n+2)})$$

This is a $(2n+1-k)$th order finite difference scheme.

Determine $f_0^{(k)}$ for an odd number k

Let $a_l + a_{-l} = 0$ and $b_l = a_l - a_{-l} = 2a_l$. It yields $a_0 = 0$ and b_1, b_2, b_3, ..., b_n satisfy

$$[b_1 + b_2 \cdot 2^k + b_3 \cdot 3^k + ... + b_n \cdot n^k] = k! \tag{8}$$

$$[b_1 + b_2 \cdot 2^j + b_3 \cdot 3^j + ... + b_n \cdot n^j] = 0 \tag{9}$$

where j is an odd number and $j \neq k$. Eqs. (8) and (9) can be rewritten as

$$\begin{bmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^3 & 3^3 & \cdots & \cdots & n^3 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ k! \\ 0 \\ \vdots \end{bmatrix} \tag{10}$$

In summary, for an *odd number* k

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^3 & 3^3 & \cdots & \cdots & n^3 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ k! \\ 0 \\ \vdots \end{bmatrix} \tag{11}$$

$a_0 = 0$, $a_{-l} = -a_l$, and

$$f_0^{(k)} = \frac{1}{h^k}\Big[\sum_{l=-n}^{+n} a_l f_l + O(h^{2n+1} f_0^{(2n+1)})\Big] = \frac{1}{h^k}\Big(\sum_{l=-n}^{+n} a_l f_l\Big) + O(h^{2n+1-k} f_0^{(2n+1)})$$

This is a $(2n-k)$th order finite difference scheme

Examples

Case 1A: $k = 1$, $n = 1$, $2n + 1 - k = 2$ (the 1st order finite difference)

$$\left[a_1\right] = \frac{1}{2}\left[1^1\right]^{-1}\left[1!\right] = \frac{1}{2}$$

$$a_{-1} = -a_1 = -1/2\,,\ a_0 = 0$$

$$f_0^{(1)} = \frac{1}{2h}(f_1 - f_{-1}) + O(h^2 f_0^{(3)})$$

Case 1B: $k = 2$, $n = 1$, $2n + 2 - k = 2$ (the 1st order finite difference)

$$\left[a_1\right] = \frac{1}{2}\left[1^2\right]^{-1}\left[2!\right] = 1$$

$$a_{-1} = a_1 = 1\,,\ a_0 = -2(a_1) = -2$$

$$f_0^{(2)} = \frac{1}{h^2}(f_1 - 2f_0 + f_{-1}) + O(h^2 f_0^{(4)})$$

Case 2A: $k=1$, $n=2$, $2n+1-k=4$ (the 3rd order finite difference)

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1^1 & 2^1 \\ 1^3 & 2^3 \end{bmatrix}^{-1}\begin{bmatrix} 1! \\ 0 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 4/3 & -1/3 \\ -1/6 & 1/6 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2/3 \\ -1/12 \end{bmatrix}$$

$a_{-1} = -a_1 = -2/3$, $a_{-2} = -a_2 = 1/12$, $a_0 = 0$

$$f_0^{(1)} = \frac{1}{h}\left(-\frac{1}{12}f_2 + \frac{2}{3}f_1 - \frac{2}{3}f_{-1} + \frac{1}{12}f_{-2}\right) + O(h^4 f_0^{(5)})$$

Case 2B: $k=2$, $n=2$, $2n+2-k=4$ (the 3rd order finite difference)

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1^2 & 2^2 \\ 1^4 & 2^4 \end{bmatrix}^{-1}\begin{bmatrix} 2! \\ 0 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 4/3 & -1/3 \\ -1/12 & 1/12 \end{bmatrix}\begin{bmatrix} 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 4/3 \\ -1/12 \end{bmatrix}$$

$$a_{-1} = a_1 = 4/3,\ a_{-2} = a_2 = -1/12,\ a_0 = -2(a_1 + a_2) = -5/2$$

$$f_0^{(2)} = \frac{1}{h^2}\left(-\frac{1}{12} f_2 + \frac{4}{3} f_1 - \frac{5}{2} f_0 + \frac{4}{3} f_{-1} - \frac{1}{12} f_{-2}\right) + O(h^4 f_0^{(6)})$$

Case 2C: $k = 3,\ n = 2,\ 2n + 1 - k = 2$ (the 1st order finite difference)

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1^1 & 2^1 \\ 1^3 & 2^3 \end{bmatrix}^{-1}\begin{bmatrix} 0 \\ 3! \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 4/3 & -1/3 \\ -1/6 & 1/6 \end{bmatrix}\begin{bmatrix} 0 \\ 6 \end{bmatrix} = \begin{bmatrix} -1 \\ +1/2 \end{bmatrix}$$

$$a_{-1} = -a_1 = 1,\ a_{-2} = -a_2 = -1/2,\ a_0 = 0$$

$$f_0^{(3)} = \frac{1}{h^3}\left(\frac{1}{2} f_2 - f_1 + f_{-1} - \frac{1}{2} f_{-2}\right) + O(h^2 f_0^{(5)})$$

Case 2D: $k = 4,\ n = 2,\ 2n + 2 - k = 2$ (the 1st order finite difference)

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1^2 & 2^2 \\ 1^4 & 2^4 \end{bmatrix}^{-1}\begin{bmatrix} 0 \\ 4! \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 4/3 & -1/3 \\ -1/12 & 1/12 \end{bmatrix}\begin{bmatrix} 0 \\ 24 \end{bmatrix} = \begin{bmatrix} -4 \\ 1 \end{bmatrix}$$

$$a_{-1} = a_1 = -4\,,\ a_{-2} = a_2 = 1,\ a_0 = -2(a_1 + a_2) = 6$$

$$f_0^{(4)} = \frac{1}{h^4}(f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}) + O(h^2 f_0^{(6)})$$

Case 3A: $k = 1,\ n = 3,\ 2n + 1 - k = 6$ (the 5th order finite difference)

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1^1 & 2^1 & 3^1 \\ 1^3 & 2^3 & 3^3 \\ 1^5 & 2^5 & 3^5 \end{bmatrix}^{-1}\begin{bmatrix} 1! \\ 0 \\ 0 \end{bmatrix}$$

$$= (\frac{1}{2})\frac{1}{120}\begin{bmatrix} 180 & -65 & 5 \\ -36 & 40 & -4 \\ 4 & -5 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{240}\begin{bmatrix} 180 \\ -36 \\ 4 \end{bmatrix} = \begin{bmatrix} 3/4 \\ -3/20 \\ 1/60 \end{bmatrix}$$

$$a_{-1} = -a_1 = -3/4\,,\ a_{-2} = -a_2 = 3/20\,,\ a_{-3} = -a_3 = -1/60\,,\ a_0 = 0$$

$$f_0^{(1)} = \frac{1}{h}\left(+\frac{1}{60}f_3 - \frac{3}{20}f_2 + \frac{3}{4}f_1 - \frac{3}{4}f_{-1} + \frac{3}{20}f_{-2} - \frac{1}{60}f_{-3}\right) + O(h^6 f_0^{(7)})$$

Benchmarks

Given

a periodic sinusoidal wave $y(x) = \sin(2\pi x / \lambda)$

or

a non-periodic step function $y(x) = \tanh(3x / w)$

Find the errors in evaluating y' ,

where

$$\text{Error} = \left| \frac{y'_{FiniteDiff} - y'_{analytic}}{\left| y'_{analytic} \right|_{\max}} \right|_{\max}$$

Table 1. Errors in Evaluating y' with $y(x) = \sin(2\pi x / \lambda)$

Grid Size Δ	0.2 λ	0.1 λ	0.01 λ	0.001 λ
5th-order FD	0.021	0.00041	4.4E-10	1.2E-12
3rd-order FD	0.069	0.0050	5.2E-07	5.3E-11
Cubic Spline	0.017	0.00091	8.7E-08	9.6E-12
1st-order FD	0.24	0.065	0.00066	6.6E-06

Table 2. Errors in Evaluating y' with $y(x) = \tanh(3x / w)$

Grid Size Δ	0.2 w	0.1 w	0.01 w	0.001 w
5th-order FD	0.022	0.00090	1.4E-09	6.1E-13
3rd-order FD	0.038	0.0036	4.3E-07	4.3E-11
Cubic Spline	0.017	0.00086	7.2E-08	7.2E-12
1st-order FD	0.10	0.029	0.00030	3.0E-06

Summary

- For finite difference scheme Error($\Delta = 0.1\lambda$)/Error($\Delta = 0.01\lambda$) $\approx 10^{m+1}$ where m is the order of the finite difference scheme.
- The 5th-order finite difference scheme with $\Delta = 0.01\lambda$ or $\Delta = 0.01$w is the best choice.
- The cubic spline provides better results at large grid size ($\Delta > 0.1\lambda$).