

0.1 Derivation of Finite Difference (FD) Approximations

0.1.1 Centered Difference for $u'(x)$

A second order finite difference approximation for $u'(x)$ at $x = \bar{x}$ is given by

$$D_0u(\bar{x}) = \frac{1}{2h}[u(\bar{x} + h) - u(\bar{x} - h)] \quad (1)$$

with an approximation for the truncation error given by the term $E(h) \approx \frac{h^2}{6}u'''(\bar{x})$.

Proof.-

Assuming that u is 4th continuously differentiable in a neighborhood of \bar{x} , the FD formula (1) and its truncation error can be obtained from Taylor expansions of u at the points $x + h$ and $x - h$. In fact,

$$u(\bar{x} - h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\beta), \quad (2)$$

$$u(\bar{x} + h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\xi), \quad (3)$$

for $\beta \in (\bar{x} - h, \bar{x})$ and $\xi \in (\bar{x}, \bar{x} + h)$. Then, by subtracting $u(\bar{x} + h) - u(\bar{x} - h)$, we obtain

$$u(\bar{x} + h) - u(\bar{x} - h) = 2hu'(\bar{x}) + \frac{h^3}{3}u'''(\bar{x}) + \mathcal{O}(h^4) \quad (4)$$

Therefore,

$$D_0u(\bar{x}) = \frac{1}{2h}[u(\bar{x} + h) - u(\bar{x} - h)] = u'(\bar{x}) + \frac{h^2}{6}u'''(\bar{x}) + \mathcal{O}(h^3) \quad (5)$$

0.1.2 Centered Difference for $u''(x)$

A second order finite difference approximation for $u''(x)$ at $x = \bar{x}$ is given by

$$D^2u(\bar{x}) = \frac{1}{h^2}[u(\bar{x} + h) - 2u(\bar{x}) + u(\bar{x} - h)] \quad (6)$$

with a truncation error given by the term $E(h) = \frac{h^4}{12}u''''(\gamma)$, where $\gamma \in (\bar{x} - h, \bar{x} + h)$.

Proof.-

Assuming that u is 4th continuously differentiable in a neighborhood of \bar{x} , the FD formula (6) and its truncation error can be obtained by adding the above Taylor expansions (2) and (3) of u at the points $x + h$ and $x - h$. In fact,

$$u(\bar{x} + h) + u(\bar{x} - h) = 2u(\bar{x}) + h^2 u''(\bar{x}) + \frac{h^4}{4!} [u''''(\xi) + u''''(\beta)] \quad (7)$$

Therefore,

$$D^2 u(\bar{x}) = \frac{1}{h^2} [u(\bar{x} + h) - 2u(\bar{x}) + u(\bar{x} - h)] = u''(\bar{x}) + \frac{h^2}{12} u''''(\gamma) \quad (8)$$

In this last step the intermediate value theorem has been used to transform the error term. In fact,

$$\frac{h^4}{4!} [u''''(\xi) + u''''(\beta)] = \frac{h^4}{12} \left[\frac{u''''(\xi) + u''''(\beta)}{2} \right] = \frac{h^4}{12} u''''(\gamma),$$

where $\gamma \in (\beta, \xi) \subset (\bar{x} - h, \bar{x} + h)$.

0.1.3 Non-Symmetric Third Order Approximation for $u'(x)$

A third order approximation $D_3 u$ for $u'(x)$ at $x = \bar{x}$ using the values of u at the neighbor points $x - 2h$, $x - h$, \bar{x} , and $x + h$, where $h > 0$ is given by

$$D_3 u(\bar{x}) = \frac{1}{3!h} [u(\bar{x} - 2h) - 6u(\bar{x} - h) + 3u(\bar{x}) + 2u(\bar{x} + h)] \quad (9)$$

with an approximation for the truncation error given by $E(h) \approx \frac{h^3}{12} u''''(\bar{x})$

Proof.-

The method of undetermined coefficients will be employed. This is $D_3 u(\bar{x})$ will be represented as

$$D_3 u(\bar{x}) = c_{-2} u(\bar{x} - 2h) + c_{-1} u(\bar{x} - h) + c_0 u(\bar{x}) + c_1 u(\bar{x} + h), \quad (10)$$

and we will determine the unknown coefficients c_i $i = -2..1$ by requiring that

$$D_3 u(\bar{x}) = u'(\bar{x}) + \mathcal{O}(h^3) \quad (11)$$

We will assume that u is 5th continuously differentiable in a neighborhood of \bar{x} , then

$$u(\bar{x} - 2h) = u(\bar{x}) - 2hu'(\bar{x}) + 4\frac{h^2}{2}u''(\bar{x}) - 8\frac{h^3}{3!}u'''(\bar{x}) + 16\frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5) \quad (12)$$

$$u(\bar{x} - h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5) \quad (13)$$

$$u(\bar{x}) = u(\bar{x}) \quad (14)$$

$$u(\bar{x} + h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5) \quad (15)$$

Substitution of these Taylor expansions into (10) leads to

$$\begin{aligned}
D_3u(\bar{x}) &= (c_{-2} + c_{-1} + c_0 + c_1)u(\bar{x}) + h(-2c_{-2} - c_{-1} + c_1)u'(\bar{x}) + \\
&\frac{h^2}{2}(4c_{-2} + c_{-1} + c_1)u''(\bar{x}) + \frac{h^3}{3!}(-8c_{-2} - c_{-1} + c_1)u'''(\bar{x}) + \\
&\frac{h^4}{4!}(16c_{-2} + c_{-1} + c_1)u''''(\bar{x}) + \mathcal{O}(h^5)
\end{aligned} \tag{16}$$

To get an approximation of $u'(\bar{x})$ of $\mathcal{O}(h^3)$ and satisfy (11), it is sufficient that

$$c_{-2} + c_{-1} + c_0 + c_1 = 0 \tag{17}$$

$$h(-2c_{-2} - c_{-1} + c_1) = 1 \tag{18}$$

$$\frac{h^2}{2}(4c_{-2} + c_{-1} + c_1) = 0 \tag{19}$$

$$\frac{h^3}{3!}(-8c_{-2} - c_{-1} + c_1) = 0 \tag{20}$$

This is a Vandermonde system of equations with matrix

$$\begin{pmatrix}
1 & 1 & 1 & 1 \\
-2h & -h & 0 & h \\
4\frac{h^2}{2} & \frac{h^2}{2} & 0 & \frac{h^2}{2} \\
-8\frac{h^3}{3!} & -\frac{h^3}{3!} & 0 & \frac{h^3}{3!}
\end{pmatrix}$$

This system has a unique solution given by

$$c_{-2} = \frac{1}{3!h}, \quad c_{-1} = \frac{-6}{3!h}, \quad c_0 = \frac{3}{3!h}, \quad c_1 = \frac{2}{3!h}$$

Therefore,

$$D_3u(\bar{x}) = \frac{1}{3!h}[u(\bar{x} - 2h) - 6u(\bar{x} - h) + 3u(\bar{x}) + 2u(\bar{x} + h)] + \mathcal{O}(h^3) \tag{21}$$

The approximation for the *truncation error* $E(h)$ is the remainder term of $\mathcal{O}(h^3)$ given by

$$E(h) \approx \frac{h^4}{4!}(16c_{-2} + c_{-1} + c_1)u''''(\bar{x}) = \frac{h^4}{4!} \frac{1}{6h}[16 - 6 + 2]u''''(\bar{x}) = \frac{h^3}{12}u''''(\bar{x}) \tag{22}$$

Table 3.1. Comparison of formulae to evaluate $d\bar{T}/dx$ at $x=1.0$

for $\bar{T}(x) = e^x$

Case	Algebraic formula	$\left[\frac{d\bar{T}}{dx}\right]_j$	Error	Leading term in T.E.
Exact	—	2.7183	—	—
3PT SYM	$(\bar{T}_{j+1} - \bar{T}_{j-1})/2\Delta x$	2.7228	0.4533×10^{-2}	0.4531×10^{-2}
FOR DIFF	$(\bar{T}_{j+1} - \bar{T}_j)/\Delta x$	2.8588	0.1406×10^{-0}	0.1359×10^{-0}
BACK DIFF	$(\bar{T}_j - \bar{T}_{j-1})/\Delta x$	2.5868	-0.1315×10^{-0}	-0.1359×10^{-0}
3PT ASYM	$(-1.5\bar{T}_j + 2\bar{T}_{j+1} - 0.5\bar{T}_{j+2})/\Delta x$	2.7085	-0.9773×10^{-2}	-0.9061×10^{-2}
5PT SYM	$(\bar{T}_{j-2} - 8\bar{T}_{j-1} + 8\bar{T}_{j+1} - \bar{T}_{j+2})/12\Delta x$	2.7183	-0.9072×10^{-5}	-0.9061×10^{-5}

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Table 3.2. Comparison of formulae to evaluate $d^2\bar{T}/dx^2$ at $x=1.0$

Case	Algebraic formula	$\left[\frac{d^2\bar{T}}{dx^2}\right]_j$	Error	Leading term in T.E.
Exact	—	2.7183	—	—
3PT SYM	$(\bar{T}_{j-1} - 2\bar{T}_j + \bar{T}_{j+1})/\Delta x^2$	2.7205	0.2266×10^{-2}	0.2265×10^{-2}
3PT ASYM	$(\bar{T}_j - 2\bar{T}_{j+1} + \bar{T}_{j+2})/\Delta x^2$	3.0067	0.2884×10^{-0}	0.2718×10^{-0}
5PT SYM	$(-\bar{T}_{j-2} + 16\bar{T}_{j-1} - 30\bar{T}_j + 16\bar{T}_{j+1} - \bar{T}_{j+2})/12\Delta x^2$	2.7183	-0.3023×10^{-5}	-0.3020×10^{-5}

Table 3.3. Truncation error leading term (algebraic): $d\bar{T}/dx$

Case	Algebraic formula	Truncation error leading term
3PT SYM	$(\bar{T}_{j+1} - \bar{T}_{j-1})/2\Delta x$	$\Delta x^2 \bar{T}_{xxx}/6$
FOR DIFF	$(\bar{T}_{j+1} - \bar{T}_j)/\Delta x$	$\Delta x \bar{T}_{xx}/2$
BACK DIFF	$(\bar{T}_j - \bar{T}_{j-1})/\Delta x$	$-\Delta x \bar{T}_{xx}/2$
3PT ASYM	$(-1.5\bar{T}_j + 2\bar{T}_{j+1} - 0.5\bar{T}_{j+2})/\Delta x$	$-\Delta x^2 \bar{T}_{xxx}/3$
5PT SYM	$(\bar{T}_{j-2} - 8\bar{T}_{j-1} + 8\bar{T}_{j+1} - \bar{T}_{j+2})/12\Delta x$	$-\Delta x^4 \bar{T}_{xxxxx}/30$

Table 3.4. Truncation error leading term (algebraic): $d^2\bar{T}/dx^2$

Case	Algebraic formula	Truncation error leading term
3PT SYM	$(\bar{T}_{j-1} - 2\bar{T}_j + \bar{T}_{j+1})/\Delta x^2$	$\Delta x^2 \bar{T}_{xxxx}/12$
3PT ASYM	$(\bar{T}_j - 2\bar{T}_{j+1} + \bar{T}_{j+2})/\Delta x^2$	$\Delta x \bar{T}_{xxx}$
5PT SYM	$(-\bar{T}_{j-2} + 16\bar{T}_{j-1} - 30\bar{T}_j + 16\bar{T}_{j+1} - \bar{T}_{j+2})/12\Delta x^2$	$-\Delta x^4 \bar{T}_{xxxxx}/90$

Table 3-1 Difference approximations using more than three points

Derivative	Finite-difference representation	Equation
$\frac{\partial^3 u}{\partial x^3} \Big _{i,j}$	$\frac{u_{i+2,j} - 2u_{i+1,j} + 2u_{i-1,j} - u_{i-2,j}}{2h^3} + O(h^2)$	(3-38)
$\frac{\partial^4 u}{\partial x^4} \Big _{i,j}$	$\frac{u_{i+2,j} - 4u_{i+1,j} + 6u_{i,j} - 4u_{i-1,j} + u_{i-2,j}}{h^4} + O(h^2)$	(3-39)
$\frac{\partial^2 u}{\partial x^2} \Big _{i,j}$	$\frac{-u_{i+3,j} + 4u_{i+2,j} - 5u_{i+1,j} + 2u_{i,j}}{h^2} + O(h^2)$	(3-40)
$\frac{\partial^3 u}{\partial x^3} \Big _{i,j}$	$\frac{-3u_{i+4,j} + 14u_{i+3,j} - 24u_{i+2,j} + 18u_{i+1,j} - 5u_{i,j}}{2h^3} + O(h^2)$	(3-41)
$\frac{\partial^2 u}{\partial x^2} \Big _{i,j}$	$\frac{2u_{i,j} - 5u_{i-1,j} + 4u_{i-2,j} - u_{i-3,j}}{h^2} + O(h^2)$	(3-42)
$\frac{\partial^3 u}{\partial x^3} \Big _{i,j}$	$\frac{5u_{i,j} - 18u_{i-1,j} + 24u_{i-2,j} - 14u_{i-3,j} + 3u_{i-4,j}}{2h^3} + O(h^2)$	(3-43)
$\frac{\partial u}{\partial x} \Big _{i,j}$	$\frac{-u_{i+2,j} + 8u_{i+1,j} - 8u_{i-1,j} + u_{i-2,j}}{12h} + O(h^4)$	(3-44)
$\frac{\partial^2 u}{\partial x^2} \Big _{i,j}$	$\frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12h^2} + O(h^4)$	(3-45)

Table 3-2 Difference approximations for mixed partial derivatives

Derivative	Finite-difference representation	Equation
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i+1,j} - u_{i+1,j-1}}{\Delta y} - \frac{u_{i,j} - u_{i,j-1}}{\Delta y} \right) + O(\Delta x, \Delta y)$	(3-46)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i,j+1} - u_{i,j}}{\Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j}}{\Delta y} \right) + O(\Delta x, \Delta y)$	(3-47)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i,j} - u_{i,j-1}}{\Delta y} - \frac{u_{i-1,j} - u_{i-1,j-1}}{\Delta y} \right) + O(\Delta x, \Delta y)$	(3-48)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j}}{\Delta y} - \frac{u_{i,j+1} - u_{i,j}}{\Delta y} \right) + O(\Delta x, \Delta y)$	(3-49)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2 \Delta y} - \frac{u_{i,j+1} - u_{i,j-1}}{2 \Delta y} \right) + O[(\Delta x, (\Delta y)^2)]$	(3-50)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{\Delta x} \left(\frac{u_{i,j+1} - u_{i,j-1}}{2 \Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2 \Delta y} \right) + O[(\Delta x, (\Delta y)^2)]$	(3-51)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{2 \Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2 \Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2 \Delta y} \right) + O[(\Delta x)^2, (\Delta y)^2]$	(3-52)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{2 \Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j}}{\Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j}}{\Delta y} \right) + O[(\Delta x)^2, \Delta y]$	(3-53)
$\frac{\partial^2 u}{\partial x \partial y} \Big _{i,j}$	$\frac{1}{2 \Delta x} \left(\frac{u_{i+1,j} - u_{i+1,j-1}}{\Delta y} - \frac{u_{i-1,j} - u_{i-1,j-1}}{\Delta y} \right) + O[(\Delta x)^2, \Delta y]$	(3-54)

Hornbeck (1975)

	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	
$2hf'(x_i) =$		-1	0	1		
$h^2f''(x_i) =$		1	-2	1		+ $O(h)^2$
$2h^3f'''(x_i) =$	-1	2	0	-2	1	
$h^4f^{(4)}(x_i) =$	1	-4	6	-4	1	

(a) Representations of $O(h)^2$

	f_{i-3}	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	f_{i+3}	
$12hf'(x_i) =$		1	-8	0	8	-1		
$12h^2f''(x_i) =$		-1	16	-30	16	-1		+ $O(h)^4$
$8h^3f'''(x_i) =$	1	-8	13	0	-13	8	-1	
$6h^4f^{(4)}(x_i) =$	-1	12	-39	56	-39	12	-1	

(b) Representations of $O(h)^4$

Fig. 3.4 Central difference representations.

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}	f_{i+5}	
$2hf'(x_i) =$	-3	4	-1				
$h^2f''(x_i) =$	2	-5	4	-1			+ $O(h)^2$
$2h^3f'''(x_i) =$	-5	18	-24	14	-3		
$h^4f^{(4)}(x_i) =$	3	-14	26	-24	11	-2	

(a) Forward difference representations

	f_{i-3}	f_{i-4}	f_{i-5}	f_{i-2}	f_{i-1}	f_i	
$2hf'(x_i) =$				1	-4	3	
$h^2f''(x_i) =$			-1	4	-5	2	+ $O(h)^2$
$2h^3f'''(x_i) =$		3	-14	24	-18	5	
$h^4f^{(4)}(x_i) =$	-2	11	-24	26	-14	3	

(b) Backward difference representations

Fig. 3.3 Forward and backward difference representations of $O(h)^2$.

FINITE DIFFERENCE FORMULAS ON NON-UNIFORM GRIDS.

We want to approximate $U^{(k)}(\bar{x})$ using a formula consisting of $n > k$ points: x_1, x_2, \dots, x_n (not necessarily uniform) and \bar{x} is not a grid point $x_i, i=1, \dots, n$.

Problem: Determine C_i ($i=1, \dots, n$) such that

$$C_1 U(x_1) + C_2 U(x_2) + \dots + C_n U(x_n) = U^{(k)}(\bar{x}) + \text{Error}. \quad (1)$$

First, consider Taylor series expansion about \bar{x} for each x_i .

$$U(x_i) = U(\bar{x}) + (\bar{x} - x_i) U'(\bar{x}) + \dots + (\bar{x} - x_i)^n U_n(\bar{x}) + \dots$$

Subst into (1) leads to

$$\begin{aligned} \left(\sum_{j=1}^n C_j \right) U(\bar{x}) + \left(\sum_{j=1}^n C_j (x_j - \bar{x}) \right) U'(\bar{x}) + \dots + \frac{1}{(n-1)!} \left(\sum_{j=1}^n C_j (x_j - \bar{x})^{n-1} \right) U^{(n-1)}(\bar{x}) \\ = U^{(k)}(\bar{x}) + \text{Error}. \end{aligned}$$

Linear system to be solved for the $C_i, i=1, \dots, n$.

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$$\begin{array}{l}
 u: \\
 u' \\
 u'' \\
 \vdots \\
 u^{(k)} \\
 \vdots \\
 u^{(n-1)}
 \end{array}
 \begin{pmatrix}
 1 & 1 & \dots & 1 \\
 \bar{x}-x_1 & \bar{x}-x_2 & \dots & \bar{x}-x_n \\
 \frac{(\bar{x}-x_1)^2}{2} & \frac{(\bar{x}-x_2)^2}{2} & \dots & \frac{(\bar{x}-x_n)^2}{2} \\
 \vdots & \vdots & \dots & \vdots \\
 \frac{(\bar{x}-x_1)^k}{k!} & \frac{(\bar{x}-x_2)^k}{k!} & \dots & \frac{(\bar{x}-x_n)^k}{k!} \\
 \vdots & \vdots & \dots & \vdots \\
 \frac{(\bar{x}-x_1)^{n-1}}{(n-1)!} & \frac{(\bar{x}-x_2)^{n-1}}{(n-1)!} & \dots & \frac{(\bar{x}-x_n)^{n-1}}{(n-1)!}
 \end{pmatrix}
 \begin{pmatrix}
 c_1 \\
 c_2 \\
 c_3 \\
 \vdots \\
 c_{k+1} \\
 \vdots \\
 c_n
 \end{pmatrix}
 =
 \begin{pmatrix}
 0 \\
 0 \\
 0 \\
 \vdots \\
 1 \\
 0 \\
 \vdots \\
 0
 \end{pmatrix}$$

Leading order error terms are given by ($k < n-1$)

$$\text{Error} = \left[\frac{1}{n!} \sum_{j=1}^n c_j (\bar{x}-x_j)^n \right] u^{(n)}(\bar{x}) + \left[\frac{1}{(n+1)!} \sum_{j=1}^n c_j (\bar{x}-x_j)^{n+1} \right] u^{(n+1)}(\bar{x})$$