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

$$D_0 u(\bar{x}) = \frac{1}{2h}[u(\bar{x}+h) - u(\bar{x}-h)] \tag{1}$$

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

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,

$$u(\bar{x}-h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u^{(4)}(\bar{x}) - \frac{h^5}{5!}u^{(5)}(\beta), \tag{2}$$

$$u(\bar{x}+h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u^{(4)}(\bar{x}) + \frac{h^5}{5!}u^{(5)}(\xi), \tag{3}$$

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

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

Therefore,

$$D_0 u(\bar{x}) = \frac{1}{2h}[u(\bar{x}+h) - u(\bar{x}-h)] = u'(\bar{x}) + \frac{h^2}{6}u'''(\bar{x}) + \mathcal{O}(h^4) \tag{5}$$

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

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

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

with a truncation error given by the term $E(h) = \dfrac{h^2}{12}u^{(4)}(\gamma)$, 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,

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

Therefore,

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

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_3u for $u'(x)$ at $x=\bar{x}$ using the values of u at the neighbor points $\bar{x}-2h$, $\bar{x}-h$, $\bar{x}$, and $\bar{x}+h$, where $h>0$ is given by

$$D_3u(\bar{x})=\frac{1}{3!h}\left[u(\bar{x}-2h)-6\,u(\bar{x}-h)+3\,u(\bar{x})+2\,u(\bar{x}+h)\right] \tag{9}$$

with an approximation for the truncation error given by $E(h)\approx\frac{h^3}{12}u^{(4)}(\bar{x})$

Proof.-

The method of undetermined coefficients will be employed. This is $D_3u(\bar{x})$ will be represented as

$$D_3u(\bar{x})=c_{-2}\,u(\bar{x}-2h)+c_{-1}\,u(\bar{x}-h)+c_0\,u(\bar{x})+c_1\,u(\bar{x}+h), \tag{10}$$

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

$$D_3u(\bar{x})=u'(\bar{x})+\mathcal{O}(h^p), \tag{11}$$

where p is the highest possible. We will assume that u is 5th continuously differentiable in a neighborhood of $\bar{x}$., then

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

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

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

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

Substitution of these Taylor expansions into (10) leads to

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

To get an approximation of $u'(\bar{x})$ of $\mathcal{O}(h^p)$ for the highest possible p, we impose the following 4 conditions for the coefficients:

$$c_{-2} + c_{-1} + c_0 + c_1 = 0 \qquad (17)$$

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

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

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

Obviously, this is the best approximation we can obtain when using 4 points (4 unknowns and 4 equations). This leads to the 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,

$$D_3u(\bar{x}) = \frac{1}{3!h}\,[u(\bar{x} - 2h) - 6\,u(\bar{x} - h) + 3\,u(\bar{x}) + 2\,u(\bar{x} + h)] + E(h). \qquad (21)$$

The approximation for the *truncation error* $E(h)$ can be computed from the last term of (16)

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

FINITE DIFFERENCE FORMULAS ON NON-UNIFORM GRIDS.

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

<u>Problem:</u> Determine c_j $(j=1,..,n)$ such that

$$c_1 u(x_1) + c_2 u(x_2) + \cdots + c_n u(x_n) = u^{(k)}(\bar{x}) + \text{Error}. \qquad (1)$$

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

$$u(x_j) = u(\bar{x}) + (x_j-\bar{x})\, u'(\bar{x}) + \cdots \frac{(x_j-\bar{x})^n}{n!} u^{(n)}(\bar{x}) + \cdots$$

Subst into (1) leads to

$$\left(\sum_{j=1}^{n} c_j\right) u(\bar{x}) + \left(\sum_{j=1}^{n} c_j (x_j-\bar{x})\right) u'(\bar{x}) + \overset{+\frac{1}{k!}\left(\sum_{j=1}^{n} c_j (x_j-\bar{x})^k\right) u^{(k)}(\bar{x}) + \cdots}{\cdots} + \frac{1}{(n-1)!}\left(\sum_{j=1}^{n} c_j (x_j-\bar{x})^{n-1}\right) u^{(n-1)}(\bar{x}) \qquad (2)$$

$$= u^{(k)}(\bar{x}) + \text{Error}.$$

Linear system to be solved for the c_j, $j=1,..,n$.

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<u>Remark:</u>

$$\text{Error} = \overset{\text{leading order term}}{\frac{1}{n!}\left(\sum_{j=1}^{n} c_j (x_j-\bar{x})^n\right) u^{(n)}(\bar{x})} + \cdots$$

In order to get the best possible approximation for $\mathcal{U}^{(k)}(\bar{x})$ $(k<n)$, we impose the conditions:

$$\sum_{j=1}^{n} c_j = 0 \; : \quad c_1 + c_2 + \dots + c_n = 0$$

$$\sum_{j=1}^{n} c_j (x_j - \bar{x}) = 0 \; : \; c_1(x_1 - \bar{x}) + c_2(x_2 - \bar{x}) + \dots + c_n(x_n - \bar{x}) = 0$$

$$\vdots$$

$$\frac{1}{k!}\sum_{j=1}^{n} c_j (x_j - \bar{x})^k = 1 \; : \; c_1 \frac{(x_1 - \bar{x})^k}{k!} + c_2 \frac{(x_2 - \bar{x})^k}{k!} + \dots + c_n \frac{(x_n - \bar{x})^k}{k!} = 1$$

$$\vdots$$

$$\frac{1}{(n-1)!}\sum_{j=1}^{n} c_j (x_j - \bar{x})^{n-1} = 0 \; : \; c_1 \frac{(x_1 - \bar{x})^{n-1}}{(n-1)!} + \dots + c_n \frac{(x_n - \bar{x})^{n-1}}{(n-1)!} = 0$$

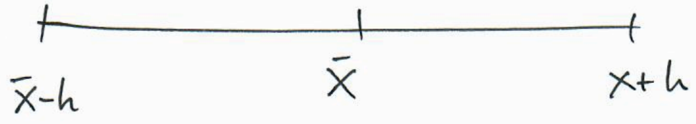
As a result, we have n equations with n unknowns: $c_1, c_2, \dots, c_n$.

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

Once $c_1, c_2, .., c_n$ have been determined the first two Leading order error terms are given by $(k<n)$

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

Derivation of centered FD approximation for $u''(\bar{x})$ using the general derivation approach



$= \text{Error}$
$= E(h)$

$$u''(\bar{x}) = \frac{u(\bar{x}-h) - 2u(\bar{x}) + u(\bar{x}+h)}{h^2} - \frac{h^2}{12} u^{(4)}(\xi)$$

$x-h < \xi < x+h$.

General derivation approach

$$\boxed{u'''(\bar{x}) \simeq c_1 u(x_1) + c_2 u(x_2) + c_3 u(x_3) + \text{Error}}$$

Taylor's Expansions around $x = \bar{x}$.

$$u(x_1) = u(\bar{x}) + (x_1-\bar{x})u'(\bar{x}) + \frac{(x_1-\bar{x})^2}{2}u''(\bar{x}) + \cdots + \frac{(x_1-\bar{x})}{!}u^{(\ )}(\bar{x})$$

$$u(x_2) = u(\bar{x}) + (x_2-\bar{x})u'(\bar{x}) + \frac{(x_2-\bar{x})^2}{2}u''(\bar{x}) + \frac{(x_2-\bar{x})^3}{3!}u'''(\bar{x}) + \frac{(x_2-\bar{x})^4}{4!}u^{(4)}(\bar{x})$$

$$u(x_3) = u(\bar{x}) + \cdots + \frac{(x_3-\bar{x})^4}{4!}u^{(4)}(\bar{x})$$

If $h_1 = x_1 - \bar{x}$, $h_2 = x_2 - \bar{x}$, $h_3 = x_3 - \bar{x}$

$$c_1 u(x_1) + c_2 u(x_2) + c_3 u(x_3) = (c_1 + c_2 + c_3) u(\bar{x})$$

$$+ (c_1 h_1 + c_2 h_2 + c_3 h_3) u'(\bar{x})$$

$$+ \left(c_1 \frac{h_1^2}{2} + c_2 \frac{h_2^2}{2} + c_3 \frac{h_3^2}{2} \right) u''(\bar{x})$$

$$+ \left(c_1 \frac{h_1^3}{3!} + c_2 \frac{h_2^3}{3!} + c_3 \frac{h_3^3}{3!} \right) u^{(3)}(\bar{x})$$

$$+ \left(c_1 \frac{h_1^4}{4!} + c_2 \frac{h_2^4}{4!} + c_3 \frac{h_3^4}{4!} \right) u^{(4)}(\bar{x}).$$

$$\overset{\text{we want}}{=} u''(\bar{x}) - \text{Error}.$$

Then, we arrive to

$$\begin{cases} c_1 + c_2 + c_3 = 0 \\ c_1 h_1 + c_2 h_2 + c_3 h_3 = 0 \\ c_1 \frac{h_1^2}{2} + c_2 \frac{h_2^2}{2} + c_3 \frac{h_3^2}{2} = 1 \end{cases}$$

This is the best possible system for the approx. because we have 3 unknowns.

<u>Augmented matrix:</u>

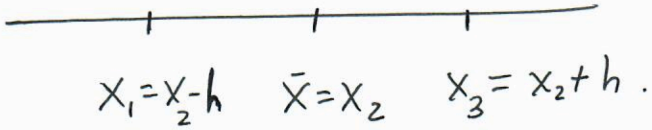
$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ h_1 & h_2 & h_3 & 0 \\ h_1^2/2 & h_2^2/2 & h_3^2/2 & 1 \end{array}\right) \sim \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & -h_1+h_2 & -h_1+h_3 & 0 \\ 0 & \frac{h_2^2}{2}-\frac{h_1^2}{2} & \frac{h_3^2}{2}-\frac{h_1^2}{2} & 1 \end{pmatrix} \frac{(h_2+h_1)}{2}(-1)$$

$$\sim \left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & h_2-h_1 & h_3-h_1 & 0 \\ 0 & 0 & \frac{h_3^2}{2}-\frac{h_1^2}{2}-(h_3-h_1)\frac{(h_2+h_1)}{2} & 1 \end{array}\right)$$

$$\boxed{C_3 = \frac{1}{(h_3-h_1)\left[\frac{h_3+h_1}{2}-\frac{h_2+h_1}{2}\right]}}$$

$$\boxed{C_2 = \frac{-(h_3-h_1)C_3}{h_2-h_1},} \quad \boxed{C_1 = -C_2 - C_3}$$

If Uniform "h_i"



then

$$h_1 = x_1 - \bar{x} = x_2 - h - x_2 = -h$$
$$h_2 = x_2 - \bar{x} = x_2 - x_2 = 0$$
$$h_3 = x_3 - \bar{x} = x_2 + h - x_2 = h.$$

$$\boxed{\begin{aligned} h_3 + h_1 &= 0 \\ h_2 + h_1 &= -h \\ h_3 - h_1 &= 2h \\ h_2 - h_1 &= h \end{aligned}}$$

Subst. into c_1, c_2 and c_3

$$C_3 = \frac{1}{2h\left(+\frac{h}{2}\right)} = \frac{1}{h^2}$$

$$C_2 = -\frac{2h}{h}\frac{1}{h^2} = -2/h^2, \quad C_1 = +\frac{2}{h^2} - \frac{1}{h^2} = \frac{1}{h^2}$$

$$\boxed{C_3 = 1/h^2}, \quad \boxed{C_2 = -\frac{2}{h^2}}, \quad \boxed{C_1 = \frac{1}{h^2}} \Rightarrow \boxed{C_1 = C_3}$$

$$\text{Error} = -\left(c_1\frac{h_1^3}{3!} + c_2\frac{h_2^3}{3!} + c_3\frac{h_3^3}{3!}\right)u^{(3)}(\bar{x}) + \left(c_1\frac{h_1^4}{4!} + c_2\frac{h_2^4}{4!} + c_3\frac{h_3^4}{4!}\right)u^{(4)}(\bar{x})$$

$$= \left(\cancel{-\frac{c_1h^3}{3} + \frac{c_3h^3}{3}}\right)^{\nearrow 0} u^{(3)}(\bar{x}) - \left(\frac{2\left(\overset{=c_1}{\frac{1}{h^2}}\right)}{4!}\right)u^{(4)}(\bar{x})$$

or $$\boxed{\text{Error} = -\frac{u^4(\bar{x})}{12}.}$$

Centered difference using three points: x_1, x_2, x_3 (arbitrary nonuniform) for $u''(\bar{x})$.

$$C_1 u(x_1) + C_2 u(x_2) + C_3 u(x_3) = u''(\bar{x}) + \text{Error}.$$

According to my notes, we need to solve the system:

$$\begin{pmatrix} 1 & 1 & 1 \\ x_1-\bar{x} & x_2-\bar{x} & x_3-\bar{x} \\ \frac{(x_1-\bar{x})^2}{2} & \frac{(x_2-\bar{x})^2}{2} & \frac{(x_3-\bar{x})^2}{2} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

If $\bar{x} = x_2$ and $x_2 - x_1 = h$, $x_3 - x_2 = h$

$$\begin{pmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ \frac{h^2}{2} & 0 & \frac{h^2}{2} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & h & 2h & 0 \\ 0 & -\frac{h^2}{2} & 0 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & h & 2h & 0 \\ 0 & 0 & h^2 & 1 \end{pmatrix}$$

$$h^2 C_3 = 1 \Rightarrow \boxed{C_3 = 1/h^2}$$

$$hC_2 = 0 - 2hC_3 = -\frac{2}{h} \Rightarrow \boxed{C_2 = -\frac{2}{h^2}}$$

$$C_1 = -C_2 - C_3 = \frac{2}{h^2} - \frac{1}{h^2} = \frac{1}{h^2} \Rightarrow \boxed{C_1 = \frac{1}{h^2}}$$

$$\therefore \boxed{\frac{1}{h^2}U_1 - \frac{2}{h^2}U_2 + \frac{1}{h^2}U_3 = u''(x_2) + \text{Error}}$$

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)

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}

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

Case	Algebraic formula	$\left[\frac{d\bar{T}^2}{dx^2}\right]_j$	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	$(\bar{T}_j - 2\bar{T}_{j+1} + T_{j+2})/\Delta x^2$	$\Delta x \bar{T}_{xxx}$
5PT SYM	$(-\bar{T}_{j-2} + 16\bar{T}_{j-1} - 30\bar{T}_j$ $+ 16\bar{T}_{j+1} - \bar{T}_{j+2})/12\Delta x^2$	$-\Delta x^4 \bar{T}_{xxxxxx}/90$

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	
$2h^3f'''(x_i) =$	-1	2	0	-2	1
$h^4f^{iv}(x_i) =$	1	-4	6	-4	1

$+ \quad \mathcal{O}(h)^2$

(*a*) Representations of $\mathcal{O}(h)^2$

	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	
$8h^3f'''(x_i) =$	1	-8	13	0	-13	8	-1
$6h^4f^{iv}(x_i) =$	-1	12	-39	56	-39	12	-1

$+ \quad \mathcal{O}(h)^4$

(*b*) Representations of $\mathcal{O}(h)^4$

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		
$2h^3f'''(x_i) =$	-5	18	-24	14	-3	
$h^4f^{iv}(x_i) =$	3	-14	26	-24	11	-2

$+ \quad \mathcal{O}(h)^2$

(*a*) Forward difference representations

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

$+ \quad \mathcal{O}(h)^2$

(*b*) Backward difference representations

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

Explanation on how to use fdcoeffF.m

1) To obtain the numerical formula for the approximation of $u^{(k)}(\bar{x})$.

In this case, we evaluate

$$\text{fdcoeffF}(K, 0, -j{:}j) \nearrow$$

Example: Find a finite diff: formula to approximate $\boxed{u''(x)}$ using $\overset{\text{arbitrary}}{}$ centered F.D.

Answ:

using fdcoeffF(2, 0, -1:1)

As a result, we get

$C(-1) = 1, \quad C(0) = -2, \quad C(1) = 1$

Then, using fdstencil.m or fdstencilRat.m

We obtain the analytical formula

$$* \frac{1}{h^2}\left[u(x_0-h) - 2u(x_0) + u(x_0+h) \right]$$

↳ Explain that we divide manually by h^k.

① If we want to evaluate

$$u''(0) \quad \text{using} \quad x_{pts} = [-1,0,1]$$

What we do is

$$\text{fdcoeffF}(2,0,-1:1) \overset{\text{dot product}}{*} \begin{bmatrix} u(-1) \\ u(0) \\ u(1) \end{bmatrix}$$

$$= c_1 u(-1) + c_2 u(0) + c_3 u(1) = u_{-1} - 2u_0 + u_1$$

② If we want to evaluate $u''(0)$ using

$$x_{pts} = [-1/2, 0, 1/2]$$

then we should do

$$\text{fdcoeffF}(2,0,[-1/2,0,1/2]) \overset{\text{dot prod.}}{*} \begin{bmatrix} u(-1/2) \\ u(0) \\ u(1/2) \end{bmatrix}$$

$$= c_1 u(-1/2) - c_2 u(0) + c_3 u(1)$$

$$= \frac{1}{(1/2)^2} u(-1/2) - \frac{2}{(1/2)^2} u(0) + \frac{1}{(1/2)^2} u(1/2)$$

$$= 4u(-1/2) - 8u(0) + 4u(1/2)$$

Run example $u''(x)$ for $u(x) = e^{x/3}$.

Explanation of fdcoeffF.m and why it gets the FD formulas when using the Vectors $k:j$ where k, j are integers. $\begin{pmatrix} k \\ k+1 \\ \vdots \\ j-1 \\ j \end{pmatrix}$

First, fdcoeffF$(k, x_b, [x_1, x_2 .., x_n])$

gives the coefficients in the formula

$$C_1 u(x_1) + C_2 u(x_2) + \cdot + C_n u(x_n) \simeq u^{(k)}(x_b)$$

Example: Compute $u^{(3)}(5)$ using 6 pts $= \begin{pmatrix} 3. \\ 3.5 \\ 5.5 \\ 6 \end{pmatrix}$

a) $$u^{(3)}(5) = C_1 u(3) + C_2 u(3.5) + C_3 u(5.5) + C_4 u(6)$$

$$= \text{fdcoeffF}(3, 5, [3, 3.5, 5.5, 6]) \cdot \begin{pmatrix} u(3) \\ u(3.5) \\ u(5.5) \\ u(6) \end{pmatrix}$$

$\downarrow$ row Vector of C_is.

If $u(x) = e^{x/3}$

$$\Rightarrow \boxed{u^{(3)}(5) \simeq 0.1690.}$$

Analytically,

$$u'(x) = \frac{1}{3} e^{x/3}, \quad u''(x) = \frac{1}{3^2} e^{x/3}, \quad u'''(x) = \frac{e^{x/3}}{3^3}.$$

$$\Rightarrow \boxed{u'''(5) = \frac{e^{5/3}}{27} = 0.1961}$$

b) Use another set of points $\begin{pmatrix}4\\4.5\\5.5\\6\end{pmatrix} = \vec{X}_{pts}$

Then

$$u^{(3)}(5) = \text{fdcoeffF}(3, 5, [4, 4.5, 5.5, 6]) \quad \begin{pmatrix}4\\4.5\\5.5\\6\end{pmatrix}$$

$\boxed{u^{(3)}(5) = 0.1975}$ vs. 0.1961
Exact.

Remark: As expected, a grid with closer points to $xb = 5$ gives better approx.

FD formulas

How to obtain (3.42) Tannehill.

$$u''(\bar{x}) = \frac{1}{h^2}\Big[2u(\bar{x}) - 5u(\bar{x}+h) + 4u(\bar{x}+2h) - u(\bar{x}+3h)\Big] \quad (2.1)$$

Using fdcoeffF.m ?

Answ: $$u''(\bar{x}) = \underset{\text{manually entered}}{\boxed{\frac{1}{h^2}}}\left[\text{fdcoeffF}(2,0,0:3) * \underset{\text{manually entered}}{\begin{pmatrix}u(\bar{x})\\u(\bar{x}+h)\\u(\bar{x}+2h)\\u(\bar{x}+3h)\end{pmatrix}}\right]$$

Why fdcoeffF(2,0,0:3) is given the right coeffs?

Because,

formula (2.1) is valid for any $\bar{x}$, in particular is valid for $\bar{x}=0$.

In this case,

$$u''(0) \simeq \frac{1}{h^2}\left[2u(0) - 5u(h) + 4u(2h) - u(3h)\right]$$

Then, if $h=1$

$$u''(0) \simeq 2u(0) - 5u(1) + 4u(2) - u(3)$$

$$\text{or } \boxed{u''(0) \simeq \begin{bmatrix} 2 & -5 & 4 & -1 \end{bmatrix} \begin{bmatrix} u(0) \\ u(1) \\ u(2) \\ u(3) \end{bmatrix}} \qquad (3.1)$$

On the other hand,

fdcoeffF(2,0,0:3) are the coeffs of $u''(0)$ using the points: 0,1,2,3 therefore $h=1$.

It means

$$\boxed{u''(0) \simeq \text{fdcoeffF}(2,0,0:3) \begin{bmatrix} u(0) \\ u(1) \\ u(2) \\ u(3) \end{bmatrix}} \qquad (3.2)$$

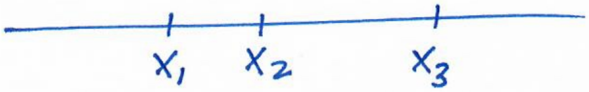
From (3.1) and (3.2) $\boxed{\text{fdcoeffF}(2,0,0:3) = [2 \ -5 \ 4 \ 1].}$

Finite Difference using Polynomial Interpolation.

Given $(x_1, \overset{u(x_1)}{v_1})$, $(x_2, \overset{u(x_2)}{v_2})$, and $(x_3, \overset{u(x_3)}{v_3})$

we want to approximate $u''(x_2) = ?$.

Non-uniform grid points



Approximating polynomial using "divided differences"

$$p(x) = a_0 + a_1(x-x_1) + a_2(x-x_1)(x-x_2)$$

$$p(x) = \underset{\underset{a_0}{\shortparallel}}{v_1} + a_1(x-x_1) + a_2(x-x_1)(x-x_2)$$

Can be expressed as

$$\boxed{p(x) = v_1 + v[x_1, x_2](x-x_1) + v[x_1, x_2, x_3](x-x_1)(x-x_2)}$$

where $\boxed{v[x_1, x_2) = \frac{v_2 - v_1}{x_2 - x_1}}$

and $\boxed{v[x_1, x_2, x_3] = \frac{v[x_2, x_3] - v[x_1, x_2]}{x_3 - x_1}}$

Details:

Interpolation polynomial for the points:

$$(x_1, v_1), \; (x_2, v_2), \; (x_3, v_3)$$

Because we have 3 distinct points, we can construct a 2nd order polynomial.

Using divide differences technique.

$$p(x) = a_0 + a_1 (x - x_1) + a_2 (x - x_1)(x - x_2)$$

The coefficients a_0, a_1, a_2 can be obtained from the interpolation points. In fact,

$$a_0: \quad v_1 = p(x_1) = a_0 \quad \Rightarrow \quad \boxed{a_0 = v_1}$$

$$a_1: \quad v_2 = p(x_2) = v_1 + a_1 (x_2 - x_1)$$

$$\Rightarrow \quad \boxed{a_1 = \frac{v_2 - v_1}{x_2 - x_1} = v[x_1, x_2]}$$

$$a_2: \; v_3 = p(x_3) = v_1 + v[x_1, x_2](x_3 - x_1)$$
$$+ a_2 (x_3 - x_1)(x_3 - x_2).$$

After some lengthy algebra

$$a_2 = \frac{\frac{v_3 - v_2}{x_3 - x_2} - \frac{v_2 - v_1}{x_2 - x_1}}{x_3 - x_1} = v[x_1, x_2, x_3].$$

Therefore,

$$p(x) = v_1 + v[x_1, x_2](x - x_1) + v[x_1, x_2, x_3](x - x_1)(x - x_2).$$

So

$$u(x) \simeq p(x), \qquad x_1 < x < x_3$$

and

$$u'(x) \simeq p'(x) = v[x_1,x_2] + \left(2x - (x_1+x_2)\right) v[x_1,x_2,x_3]$$

and

$$\boxed{u''(x) \simeq p''(x) = 2v[x_1,x_2,x_3], \quad \text{Constant}} \quad (2.1)$$

In particular,

$$u''(x_2) = 2v[x_1,x_2,x_3]$$

If $\boxed{h_1 = x_2 - x_1}$, $\boxed{h_2 = x_3 - x_2}$

then,

$$v[x_1,x_2,x_3] = \frac{\dfrac{v_3 - v_2}{h_2} - \dfrac{v_2 - v_1}{h_1}}{h_2 + h_1}$$

$$= \frac{v_3}{h_2(h_2+h_1)} - \frac{1}{h_1 h_2} v_2 + \frac{v_1}{h_1(h_2+h_1)}$$

Thus,

$$\boxed{u''(x_2) \simeq p''(x_2) = \frac{2u(x_1)}{h_1(h_2+h_1)} - \frac{2u(x_2)}{h_1 h_2} + \frac{2u(x_3)}{h_2(h_2+h_1)}}$$

(2.2)

Computation of error:

Expanding $u(x_1)$ and $u(x_3)$ in Taylor series about x_2

$$u(x_1) = u(x_2) + \overset{-h_1}{(x_1-x_2)}\, u'(x_2) + \frac{\overset{h_1^2}{(x_1-x_2)^2}}{2}\, u''(x_2) + \frac{\overset{-h_1^3}{(x_1-x_2)^3}}{3!}\, u'''(x_2) + \frac{\overset{h_1^4}{(x_1-x_2)^4}}{4!}\, u^{(4)}(x_2) + \cdots$$

$$u(x_3) = u(x_2) + h_2\, u'(x_2) + \frac{h_2^2}{2}\, u''(x_2) + \frac{h_2^3}{3!}\, u^{(3)}(x_2) + \frac{h_2^4}{4!}\, u^{(4)}(x_2) + \cdots$$

then,

$$p''(x_2) = \Big(\overbrace{\frac{2}{h_1(h_2+h_1)} + \frac{2}{h_2(h_1+h_2)} - \frac{2}{h_1 h_2}}^{=0}\Big)\, u(x_2)$$

$$+ \Big(\overbrace{\frac{-2h_1}{h_1(h_2+h_1)} + \frac{2h_2}{h_2(h_2+h_1)}}^{=0}\Big)\, u'(x_2) +$$

$$+ \Big(\overbrace{\frac{2h_1^2}{2h_1(h_2+h_1)} + \frac{2h_2^2}{2h_2(h_1+h_2)}}^{=1}\Big)\, u''(x_2)$$

$$+\left(\frac{-2h_1^3}{3!\,h_1(h_2+h_1)}+\frac{2h_2^3}{3!\,h_2(h_1+h_2)}\right)u'''(x_2)$$

$$+\left(\frac{2h_1^4}{4!\,h_1(h_2+h_1)}+\frac{2h_2^4}{4!\,h_2(h_1+h_2)}\right)u^{(4)}(x_2)+\cdots$$

$$=u''(x_2)+\frac{1}{3}(h_2-h_1)\,u'''(x_2)+\frac{1}{12}\left(\frac{h_1^3+h_2^3}{h_1+h_2}\right)u^{(4)}(x_2)$$

Therefore, Truncation error.

$$\boxed{p''(x_2)-u''(x_2)=\frac{1}{3}(h_2-h_1)\,u'''(x_2)+\frac{1}{12}\left(\frac{h_1^3+h_2^3}{h_1+h_2}\right)u^{(4)}(x_2)} \qquad (4.1)$$

If $h_1=h_2=h$, $x_1=x_2-h$, $x_3=x_2+h$

$$u''(x_2)\simeq p(x_2)=\frac{2}{2h^2}u(x_1)-\frac{2}{h^2}u(x_2)+\frac{2}{2h^2}u(x_3)$$

Then, Substitution into (2.2)

$$u''(x_2)\simeq\frac{u(x_3)-2u(x_2)+u(x_1)}{h^2}.$$

or

$$\boxed{u''(x_2)=\frac{u(x_2+h)-2u(x_2)+u(x_2-h)}{h^2}}$$

Same as centered finite difference approximation of $u''(x_2)$ previously obtained.

(I)

$$u(x_2):\ \frac{2}{h_1(h_2+h_1)} + \frac{2}{h_2(h_1+h_2)} - \frac{2}{h_1h_2} =$$

$$\frac{2\cancel{(h_2+h_1)}}{h_1h_2\cancel{(h_1+h_2)}} - \frac{2}{h_1h_2} = 0. \ ✓$$

(II) $$u'(x_2):\ \frac{-2h_1}{h_1(h_2+h_1)} + \frac{2h_2}{h_2(h_2+h_1)} = \frac{-2h_1h_2+2h_2h_1}{h_1h_2(h_2+h_1)} = 0 \ ✓$$

(III) $$u''(x_2):\ \frac{2h_1^2}{2h_1(h_2+h_1)} + \frac{2h_2^2}{2h_2(h_2+h_1)} = \frac{2h_1^2h_2+2h_2^2h_1}{2h_1h_2(h_2+h_1)} = 1 \ ✓$$

(IV) $$u'''(x_2):\ \frac{-2h_1^3}{3!\,h_1(h_2+h_1)} + \frac{2h_2^3}{3!\,h_2(h_2+h_1)} = \frac{2h_2^3h_1-2h_1^3h_2}{3!\,h_1h_2(h_2+h_1)}$$

$$= \frac{2\cancel{h_1h_2}(h_2^2-h_1^2)}{3!\,\cancel{h_1h_2}(h_2+h_1)}$$

$$= \frac{1}{3}\frac{(h_2-h_1)\cancel{(h_2+h_1)}}{\cancel{(h_2+h_1)}} = \frac{1}{3}(h_2-h_1). \ ✓$$

(V) $$u^{(4)}(x_2):\ \frac{2h_1^4}{4!\,h_1(h_2+h_1)} + \frac{2h_2^4}{4!\,h_2(h_2+h_1)} = \frac{2h_1^4h_2+2h_2^4h_1}{4!\,h_1h_2(h_2+h_1)}$$

$$= \frac{\cancel{h_1h_2}(h_1^3+h_2^3)}{12\,\cancel{h_1h_2}(h_2+h_1)} = \frac{h_1^3+h_2^3}{12(h_2+h_1)} \ ✓$$

and the $\overset{T.E.}{\text{error}}$ reduces to

$$T.E. = \frac{1}{3}(0)\, u'''(x_2) + \frac{1}{12}\frac{2h^3}{2h}\, u^{(4)}(x_2)$$

or

$$\boxed{T.E. = p''(x_2) - u''(x_2) = \frac{h^2}{12}\, u^{(4)}(x_2).} \qquad (5.1).$$

Same as truncation error (1.13) for centered finite difference approximation of $u''(x_2)$ in Leveque's book.