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 $E(h) \approx \frac{h^2}{6}u'''(\bar{x})$.

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,

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

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

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

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

Therefore,

$$D_0 u(\bar{x}) = \frac{1}{2h}[u(\bar{x}+h) - u(\bar{x}-h)] = u'(\bar{x}) + \frac{h^2}{6}u'''(\bar{x}) + \mathcal{O}(h^3) \tag{5}$$

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 $E(h) = \frac{h^4}{12}u''''(\gamma)$, 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,

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

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 $x-2h$, $x-h$, $\bar{x}$, and $x+h$, 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 $E(h)\approx\dfrac{h^3}{12}u''''(\bar{x})$

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

$$D_3u(\bar{x})=u'(\bar{x})+\mathcal{O}(h^3) \tag{11}$$

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

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

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

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

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

Substitution of these Taylor expansions into (10) leads to

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

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 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,

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

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

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