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

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

$$u(\bar{x} - h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2} u''(\bar{x}) - \frac{h^3}{3!} u'''(\bar{x}) + \frac{h^4}{4!} u'''(\beta),$$  \hspace{1cm} (2)

$$u(\bar{x} + h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2} u''(\bar{x}) + \frac{h^3}{3!} u'''(\bar{x}) + \frac{h^4}{4!} u'''(\xi),$$  \hspace{1cm} (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

$$u(\bar{x} + h) - u(\bar{x} - h) = 2hu'(\bar{x}) + \frac{h^3}{3} u'''(\bar{x}) + O(h^4)$$  \hspace{1cm} (4)

Therefore,

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

$$D^2 u(\bar{x}) = \frac{1}{h^2} [u(\bar{x} + h) - 2u(\bar{x}) + u(\bar{x} - h)]$$  \hspace{1cm} (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 \( ar{x} \), 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,
\[
 u(x + h) + u(x - h) = 2u(x) + h^2u''(x) + \frac{h^4}{4!} [u'''(\xi) + u'''(\beta)]
\]
(7)
Therefore,
\[
 D^2u(x) = \frac{1}{h^2} [u(x + h) - 2u(x) + u(x - h)] = u''(x) + \frac{h^2}{12}u'''(\gamma)
\]
(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 \( \gamma \in (\beta, \xi) \subset (x - h, \bar{x} + h) \).

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
\[
 D_3u(\bar{x}) = \frac{1}{3!h} [u(\bar{x} - 2h) - 6u(\bar{x} - h) + 3u(\bar{x}) + 2u(\bar{x} + h)]
\]
(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 \( D_3u(\bar{x}) \) will be represented as
\[
 D_3u(\bar{x}) = c_{-2} u(\bar{x} - 2h) + c_{-1} u(\bar{x} - h) + c_0 u(\bar{x}) + c_1 u(\bar{x} + h),
\]
(10)
and we will determine the unknown coefficients \( c_i i = -2..1 \) by requiring that
\[
 D_3u(\bar{x}) = u'(\bar{x}) + O(h^3)
\]
(11)
We will assume that \( u \) is 5th continuously differentiable in a neighborhood of \( \bar{x} \), then
\[
 u(\bar{x} - 2h) = u(\bar{x}) - 2hu'(\bar{x}) + \frac{h^2}{2} u''(\bar{x}) - \frac{8h^3}{3!} u'''(\bar{x}) + 16\frac{h^4}{4!} u''''(\bar{x}) + O(h^5)
\]
(12)
\[
 u(\bar{x} - h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2} u''(\bar{x}) - \frac{h^3}{3!} u'''(\bar{x}) + \frac{h^4}{4!} u''''(\bar{x}) + O(h^5)
\]
(13)
\[
 u(\bar{x}) = u(\bar{x})
\]
(14)
\[
 u(\bar{x} + h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2} u''(\bar{x}) + \frac{h^3}{3!} u'''(\bar{x}) + \frac{h^4}{4!} u''''(\bar{x}) + O(h^5)
\]
(15)
Substitution of these Taylor expansions into (10) leads to

\[ D_3 u(\bar{x}) = (c_{-2} + c_{-1} + c_0 + c_1)u(\bar{x}) + h (-2c_{-2} - c_{-1} + c_1)u'(\bar{x}) + \]
\[ \frac{h^2}{2} (4c_{-2} + c_{-1} + c_1)u''(\bar{x}) + \frac{h^3}{3!} (-8c_{-2} - c_{-1} + c_1)u'''(\bar{x}) + \]
\[ \frac{h^4}{4!} (16c_{-2} + c_{-1} + c_1)u''''(\bar{x}) + \mathcal{O}(h^5) \] 

(16)

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

\[ c_{-2} + c_{-1} + c_0 + c_1 = 0 \] 

(17)

\[ h (-2c_{-2} - c_{-1} + c_1) = 1 \] 

(18)

\[ \frac{h^2}{2} (4c_{-2} + c_{-1} + c_1) = 0 \] 

(19)

\[ \frac{h^3}{3!} (-8c_{-2} - c_{-1} + c_1) = 0 \] 

(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,

\[ D_3 u(\bar{x}) = \frac{1}{3!h} [u(\bar{x} - 2h) - 6 u(\bar{x} - h) + 3 u(\bar{x}) + 2 u(\bar{x} + h)] + \mathcal{O}(h^3) \] 

(21)

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

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

(22)