4.0. Introduction

In the conventional calculus the operation of differentiation of a function is a well-defined, formal procedure with the operations highly dependent upon the form of the function involved. Many different types of rules are needed for different functions. In numerical (approximate) methods a digital computer is employed which can only perform the standard arithmetic operations of addition, subtraction, multiplication, division, exponentiation and certain logical operations. We thus need a technique for (approximately) differentiating functions by employing only arithmetic operations. The finite difference calculus satisfies this need.

4.1. Forward Differences in One Dimension

Consider a function \( f(x) \) that is analytic\(^1\) in the neighborhood of a point \( x = c \) as shown in Figure 4.1.

\( f(x) \)

\[ h \quad h \quad h \]

\[ c - h \quad x = c \quad c + h \]

\( \text{actual slope} \)

---

\(^1\) If a function \( f(x) \) possesses a derivative at \( x = c \) and at every point in some neighborhood of \( c \), the \( f(x) \) is said to be analytic at \( c \) and \( c \) is called a regular point of the function [2].
**Figure 4.1.** Schematic Representation of the Slope at \( x = c \).

We seek an approximation for \( f'(x) \mid_{x=c} ; c \in [a,b] \). Begin by determining an expression for \( f(c + h) \). This is achieved by expanding \( f(c + h) \) in a Taylor series about \( c \)

\[
f(c + h) = f(c) + hf'(c) + \frac{h^2}{2!} f''(c) + \frac{h^3}{3!} f'''(c) + \cdots \tag{4.1}
\]

Solving equation (4.1) for \( f'(c) \) gives

\[
f'(c) = \frac{f(c + h) - f(c)}{h} - \frac{h}{2} f''(c) - \frac{h^2}{6} f'''(c) - \cdots \tag{4.2}
\]

or

\[
f'(x) \mid_{x=c} = \frac{f(c + h) - f(c)}{h} + O(h) \tag{4.3}
\]

Equation (4.3) represents an expression for \( f'(x) \) at \( x = c \) that is accurate within an error of \( h \). Graphically the expression \( \frac{f(c + h) - f(c)}{h} \) approximates the slope of \( f \) at the point \( x = c \) by the slope of the straight line passing through \( f(c + h) \) and \( f(c) \); i.e.,

**Figure 4.2.** Forward Difference Approximation to the Slope at \( x = c \).

Clearly, as \( h \) is reduced, the approximate slope approaches the exact one. For convenience and brevity, the following subscript notation is adopted

\[
f(x) \mid_{x=c} \equiv f_j \tag{4.4}
\]
Define the forward difference of $f$ at $j$ as

$$\Delta f_j \equiv f_{j+1} - f_j \quad (4.6)$$

Equation (4.3) can thus be written as

$$f'(x) \big|_{x = c} = \frac{\Delta f_j}{h} + \mathcal{O}(h) \quad (4.7)$$

Having derived an approximate expression for $f'(x) \big|_{x = c}$, $c \in [a, b]$, attention is now turned to determining approximations to higher order derivatives. Recall the Taylor series expansion for $f(x) \big|_{x = c + h}$ given by equation (4.1). An expression for $f(x) \big|_{x = c + 2h}$ is obtained by performing a similar expansion; i.e.,

$$f(c + 2h) = f(c) + 2hf'(c) + 2h^2f''(c) + \frac{4h^3}{3}f'''(c) + \cdots \quad (4.8)$$

Subtracting two times equation (4.1) from equation (4.8) drops out the $f'(c)$ terms, giving

$$f(c + 2h) - 2f(c + h) = -f(c) + h^2f''(c) + h^3f'''(c) + \cdots \quad (4.9)$$

Solving for $f''(c)$, and using the subscript notation, gives

$$f''(x) \big|_{x = c} = \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + \mathcal{O}(h) \quad (4.10)$$

Defining the second forward difference of $f$ at $j$ as

$$\Delta^2 f_j \equiv f_{j+2} - 2f_{j+1} + f_j \quad (4.11)$$

It follows that

$$f''(x) \big|_{x = c} = \frac{\Delta^2 f_j}{h^2} + \mathcal{O}(h) \quad (4.12)$$
In general, any forward difference may be obtained by starting from the first difference and by using the following recurrence formula

\[ \Delta^n f_j = \Delta_f \left( \Delta^{n-1} f_j \right) \]  
(4.13)

That is, any order forward difference can be obtained by taking the forward differences of the next lower forward differences. In general, the forward difference expression for derivatives of \textit{any} order is given by

\[ \left. \frac{d^n f}{dx^n} \right|_{x=c} = \frac{\Delta^n f_j}{h^n} + O(h) \]  
(4.14)

**Example 4.1.** Forward difference \( O(h) \) for the third derivative of a function.

Consider the case with \( n = 3 \). It follows from equation (4.13) that

\[ \Delta^3 f_j = \Delta_f \left\{ \Delta^2 f_j \right\} = \Delta_f \left\{ \Delta_f \left\{ \Delta_f f_j \right\} \right\} \]  
(1)
\[ = \Delta_f \left\{ \Delta_f \{ f_{j+1} - f_j \} \right\} = \Delta_f \left\{ \Delta_f f_{j+1} - \Delta_f f_j \right\} \]
\[ = \Delta_f \left\{ (f_{j+2} - f_{j+1}) - (f_{j+1} - f_j) \right\} = \Delta_f \left\{ f_{j+2} - 2f_{j+1} + f_j \right\} \]
\[ = (f_{j+3} - f_{j+2}) - 2(f_{j+2} - f_{j+1}) + (f_{j+1} - f_j) = f_{j+3} - 3f_{j+2} + 3f_{j+1} - f_j \]

Then according to equation (4.14)

\[ \left. \frac{d^3 f}{dx^3} \right|_{x=c} = \frac{\Delta^3 f_j}{h^3} + O(h) = \frac{f_{j+3} - 3f_{j+2} + 3f_{j+1} - f_j}{h^3} + O(h) \]  
(2)

Forward difference approximations to the first four derivatives are given in Table 4.1.
Table 4.1. Forward Difference Representations of O(h)

The above forward differences are all $O(h)$. However, by including more terms in the Taylor series expansion, expressions of greater accuracy may be obtained. For example, from equation (4.2) it follows that

$$f'(c) = \frac{f(c + h) - f(c)}{h} = \frac{h}{2} f''(c) + \frac{h^2}{6} f'''(c) - \cdots$$  \hspace{1cm} (4.15)

The approximation to $f''(x)|_{x=c}$ is given by equation (4.10), which is now written in the form

$$f''(c) = \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} - hf'''(c)$$  \hspace{1cm} (4.16)

Substituting equation (4.16) into equation (4.15), and using exclusively subscript notation gives

$$f'(x)|_{x=c} = \frac{f_{j+1} - f_j}{h} - \frac{f_{j+2} - 2f_{j+1} + f_j}{2h} + \frac{h^2}{3} f'''(c) + \cdots$$  \hspace{1cm} (4.17)

or

$$f'(x)|_{x=c} = -\frac{f_{j+2} + 4f_{j+1} - 3f_j}{2h} + O(h)^2$$  \hspace{1cm} (4.18)

Additional higher order forward differences are summarized in Table 4.2.
Selected Topics in Numerical Analysis

<table>
<thead>
<tr>
<th>2h ( f'(x_j) = )</th>
<th>2h ( f''(x_j) = )</th>
<th>2h ( f'''(x_j) = )</th>
<th>2h ( f^iv(x_j) = )</th>
</tr>
</thead>
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<td>-5</td>
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</tr>
<tr>
<td>3</td>
<td>-14</td>
<td>26</td>
<td>-24</td>
</tr>
</tbody>
</table>

+ \( O(h^2) \)

**Table 4.2. Forward Difference Representations of \( O(h^2) \)**

Observe from Tables 4.1 and 4.2 that for a given approximation (i.e., a given row in the tables), the coefficients sum to zero. Why must this be so? 2

### 4.2. Backward Differences in One Dimension

Consider an expression for \( f(c - h) \) by using a Taylor series expansion of \( f(c) \) about the point \( x = c \)

\[
f(c - h) = f(c) - hf'(c) + \frac{h^2}{2!} f''(c) - \frac{h^3}{3!} f'''(c) + \cdots \tag{4.19}
\]

Solving for \( f'(c) \) gives

\[
f'(c) = \frac{f(c) - f(c - h)}{h} + \frac{h}{2} f''(c) - \frac{h^2}{6} f'''(c) + \cdots \tag{4.20}
\]

or

\[
f'(x)|_{x=c} = \frac{f_j - f_{j-1}}{h} + O(h) \tag{4.21}
\]

Define the *first backward difference* of \( f \) at \( j \) as

---

2 The coefficients associated with any finite difference approximation must add up to zero so that if a function is constant over \([a, b]\), the first (and subsequent) derivative must be exactly zero.
\[ \Delta_B f_j \equiv f_j - f_{j-1} \]  

(4.22)

It follows, therefore, that

\[ f'(x) \big|_{x=c} = \frac{\Delta_B f_j}{h} + O(h) \]  

(4.23)

The graphical interpretation of the first backward difference of \( f \) at \( j \) is the slope of the straight line connecting \( f(x) \big|_{x=c} \) and \( f(x) \big|_{x=c+h} \). That is,

\[ hhf(x) \]
\[ \text{backward difference approximation} \]
\[ c \quad c \quad c + h \]
\[ \text{actual slope} \]

Figure 4.3. Backward Difference Approximation to the Slope at \( x = c \).

Approximations to higher order derivatives using backward differences are obtained in a manner similar to that for forward differences. By using equation (4.19) along with a similar expansion about \( c \) to obtain \( f(c-2h) \), the following backward difference expression for \( f''(x) \) at \( x = c \) is obtained:

\[ f''(x) \big|_{x=c} = \frac{f_j - 2f_{j-1} + f_{j-2}}{h^2} + O(h) \]  

(4.24)

or

\[ f''(x) \big|_{x=c} = \frac{\Delta_B^2 f_j}{h^2} + O(h) \]  

(4.25)

In general, any backward difference may be obtained by starting from the first backward difference and by using the following recurrence formula
\[ \Delta_{B}^{n} f_{j} \equiv \Delta_{B} \left( \Delta_{B}^{n-1} f_{j} \right) \]  

(4.26)

That is, any order backward difference can be obtained by taking the backward differences of the next lower backward differences.

In general, the backward difference expression for derivatives of any order is given by

\[
\frac{d^{n} f}{dx^{n}} \bigg|_{x=c} = \frac{\Delta_{B}^{n} f_{j}}{h^{n}} + O(h) 
\]

(4.27)

Approximations to the first four derivatives are given in Table 4.3.

| \hline
| \hline
| \hline
| \hline
| \hline

\[
\begin{array}{ccccc}
 f_{j-4} & f_{j-3} & f_{j-2} & f_{j-1} & f_{j} \\
 h f'(x_{j}) = & & -1 & 1 & \\
h^{2} f''(x_{j}) = & 1 & -2 & 1 & + O(h) \\
h^{3} f'''(x_{j}) = & -1 & 3 & -3 & 1 \\
h^{4} f^{iv}(x_{j}) = & 1 & -4 & 6 & -4 & 1 \\
\end{array}
\]

Table 4.3. Backward Difference Representations of O(h)

Higher order backward differences are obtained by simply taking more terms in the Taylor series expansion. An example of a higher order backward difference approximation for \( f'(x) \big|_{x=c} \) is

\[
f'(x) \big|_{x=c} = \frac{3f_{j} - 4f_{j-1} + f_{j-2}}{2h} + O(h)^{2}
\]

(4.28)

Additional higher order backward differences are summarized in Table 4.4.
39

**Table 4.4.** Backward Difference Representations of \( O(h)^2 \)

### 4.3. Central Differences in One Dimension

Consider once again the analytic function \( f(x) \) shown in Figure 4.1. The forward and backward Taylor series expansions about \( x = c \) are respectively

\[
f(c + h) = f(c) + hf'(c) + \frac{h^2}{2!} f''(c) + \frac{h^3}{3!} f'''(c) + \cdots \quad (4.29)
\]

\[
f(c - h) = f(c) - hf'(c) + \frac{h^2}{2!} f''(c) - \frac{h^3}{3!} f'''(c) + \cdots \quad (4.30)
\]

Subtracting equation (4.30) from equation (4.29) cancels the even powers of \( h \), giving

\[
f(c + h) - f(c - h) = 2hf'(c) + \frac{h^3}{3} f'''(c) + \cdots \quad (4.31)
\]

Solving for \( f'(c) \) gives

\[
f'(c) = \frac{f(c + h) - f(c - h)}{2h} - \frac{h^2}{6} f'''(c) - \cdots \quad (4.32)
\]

or
This difference representation, which is accurate to $O(h^2)$, is called the *central difference representation* of $f'(x)$ at $x_j$. Note that the point $x_j$ itself is not involved, and that from the error term in equation (4.32), this expression is exact for polynomials of degree 2 (i.e., parabolas) and lower. Graphically, the central difference representation of $f$ at $x$ is the slope of the straight line from $f_{j-1}$ to $f_{j+1}$ (see Figure 4.4).

![Figure 4.4. Central Difference Approximation to the Slope at $x = c$.](image)

To obtain an expression for $f''(x)|_{x=c}$ that is $O(h^2)$, add equations (4.29) and (4.30). The results is

$$f(c + h) + f(c - h) = 2f(c) + h^2 f''(c) + \frac{h^4}{12} f^{iv}(c) + \cdots$$

or

$$f''(c) = \frac{f(c + h) - 2f(c) + f(c - h)}{h^2} - \frac{h^2}{12} f^{iv}(c) - \cdots$$

Finally, using subscript notation, the central difference representation for $f''(x)$ at $x_j$ is given by

$$f''(x)|_{x=c} = \frac{f_{j+1} - 2f_{j} + f_{j-1}}{h^2} + O(h^2)$$

(4.36)
In general, the value of \( f_j \) appears only in representations of even derivatives. This is summarized in the following expressions

\[
\frac{d^n f}{dx^n}
\bigg|_{x=x_j} = \frac{\Delta^n_B f_{j+0.5n} + \Delta^n_F f_{j-0.5n}}{2h^n} + \mathcal{O}(h)^2 \quad ; \quad n \text{ even} \quad (4.37)
\]

\[
\frac{d^n f}{dx^n}
\bigg|_{x=x_j} = \frac{\Delta^n_B f_{j+0.5(n-1)} + \Delta^n_F f_{j-0.5(n-1)}}{2h^n} + \mathcal{O}(h)^2 \quad ; \quad n \text{ odd} \quad (4.38)
\]

Central difference approximations \( \mathcal{O}(h)^2 \) and \( \mathcal{O}(h)^d \) to the first four derivatives are given in Tables 4.5 and 4.6, respectively.

<table>
<thead>
<tr>
<th>( f_{j-2} )</th>
<th>( f_{j-1} )</th>
<th>( f_j )</th>
<th>( f_{j+1} )</th>
<th>( f_{j+2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2h ( f' (x_j) = )</td>
<td>(-1)</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>( h^2 f'' (x_j) = )</td>
<td>1</td>
<td>(-2)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2h ( 3f''' (x_j) = )</td>
<td>(-1)</td>
<td>2</td>
<td>0</td>
<td>(-2)</td>
</tr>
<tr>
<td>( h^4 f^iv (x_j) = )</td>
<td>1</td>
<td>(-4)</td>
<td>6</td>
<td>(-4)</td>
</tr>
</tbody>
</table>

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

**Table 4.5.** Central Difference Representations of \( \mathcal{O}(h)^2 \)
4.4. Finite Differences in Two Dimensions

Although the problem of approximating differential equations in two or more independent variables is more involved than for the case involving approximation in one variable. Using Taylor’s theorem for a function of two variables yields the following results (NOTE: the subscript notation \( f(x_i, y_j) \equiv f_{i,j} \) and \( h \equiv x_{i+1} - x_i \) is used in the sequel):

- A forward difference approximation for \( \frac{\partial f}{\partial x_{i,j}} \) :

\[
\frac{\partial f}{\partial x_{i,j}} \bigg|_{i,j} = \frac{f_{i+1,j} - f_{i,j}}{h} + O(h) \quad (4.39)
\]

- A backward difference approximation for \( \frac{\partial f}{\partial x_{i,j}} \) :

\[
\frac{\partial f}{\partial x_{i,j}} \bigg|_{i,j} = \frac{f_{i,j} - f_{i-1,j}}{h} + O(h) \quad (4.40)
\]
• A central difference approximation for \( \frac{\partial f}{\partial x}_{i,j} \):

\[
\frac{\partial f}{\partial x}_{i,j} = \frac{f_{i+1,j} - f_{i-1,j}}{2h} + O(h^2) \tag{4.41}
\]

• A central difference approximation for \( \frac{\partial^2 f}{\partial x^2}_{i,j} \):

\[
\frac{\partial^2 f}{\partial x^2}_{i,j} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h^2} + O(h^2) \tag{4.42}
\]

Similar expressions can be obtained for difference approximations of \( \frac{\partial f}{\partial y}_{i,j} \) and \( \frac{\partial^2 f}{\partial y^2}_{i,j} \).
4.5. References
