3.1 Finite Difference Approximations

Consider the discrete-valued function shown in **Figure 3.1**. The material covered in this section will show how to estimate the first and second derivatives at any of the data points using only the function values at the discrete points.

We begin this section with a review of the Taylor series expansion since it is the basis for our finite difference approximations. First, consider a function of a single variable, shown in **Figure 3.2**. Then the Taylor series expansion for $f(x)$ near $x = x_0$ is given as

$$f(x) = f(x_0) + (x - x_0)\, f'(x_0) + \frac{(x - x_0)^2}{2} f''(x_0) + \frac{(x - x_0)^3}{6} f'''(x_0) + \sum_{n=4}^{\infty} \frac{(x - x_0)^n}{n!} f^n(x_0) \tag{3.1}$$

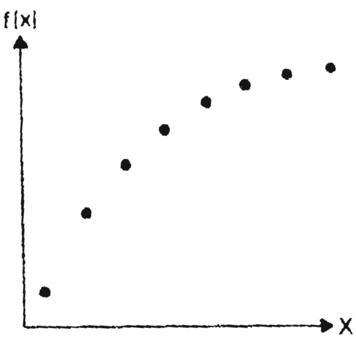

Figure 3.1 Discrete-valued function.

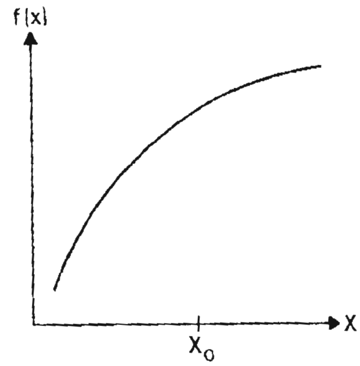

Figure 3.2 Function of a single variable.

Note that

$$f'(x_0) = \left.\frac{df}{dx}\right|_{x = x_0}, \quad f''(x_0) = \left.\frac{d^2 f}{dx^2}\right|_{x = x_0}, \quad \ldots, \quad f^n(x_0) = \left.\frac{d^n f}{dx^n}\right|_{x = x_0}$$

Also note that all the derivatives are evaluated at $x = x_0$.

Example 3.1 Taylor Series Expansion

Problem Statement

Use the Taylor series expansion (**Equation 3.1**) to estimate $e^{1.1}$ using function and derivative values of e^{x_0} where $x_0 = 1.0$.

Solution

Applying the Taylor series expansion to e^x about $x_0 = 1.0$ yields

$$e^x = e + (x - 1)\, e + \frac{(x - 1)^2}{2} e + \frac{(x - 1)^3}{6} e + \cdots$$

since

$$\frac{d^n}{dx^n}(e^x) = e^x$$

Table 3.1 shows the approximation of $e^{1.1}$ for an increasing number of terms used in the Taylor series expansion. Note that, as more terms are used in the Taylor series expansion, the approximation approaches the exact value.

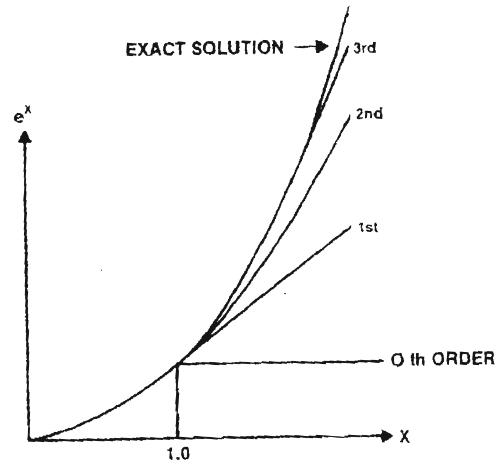

Figure 3.3 0th, 1st, 2nd, and 3rd order approximations of e^x about $x = 1.0$.

Table 3.1 The Effect of Using an Increasing Number of Terms in a Taylor Series Expansion

Approximation Order	Value of the Approximation	Difference between Analytical Value and the Approximation
0th Order	2.71828	2.86×10^{-1}
1st Order	2.99011	1.41×10^{-2}
2nd Order	3.00370	4.65×10^{-4}
3rd Order	3.00415	1.56×10^{-5}

Figure 3.3 shows the zeroth order, first order, second order, and third order approximations of e^x about $x_0 = 1.0$. The zeroth order approximation uses only the first term in the Taylor series expansion. The first order approximation uses the first two terms, and the second order and third order approximations use the first three and four terms, respectively.

Figure 3.4 shows graphically the forward difference, backward difference, and central difference approximation of the first derivative. Consider the Taylor series expansion for $f(x_{i+1})$ about $x = x_i$, i.e.,

$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + \cdots$$

where

$$\Delta x = x_{i+1} - x_i$$

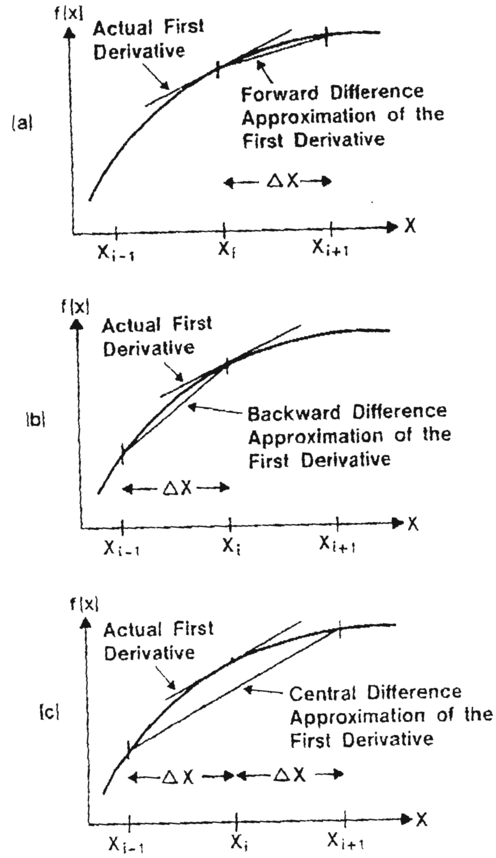

Figure 3.4 (a) Forward, (b) backward, and (c) central difference approximation of the first derivative.

Solving for $f'(x_i)$ yields

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{\Delta x}{2} f''(x_i) - \frac{\Delta x^2}{6} f'''(x_i) + \cdots$$

This result is shown graphically in **Figure 3.4a** as the forward difference approximation of the first derivative. Note that the error of this approximation is given by

$$-\frac{\Delta x}{2} f''(x_i) - \frac{\Delta x^2}{6} f'''(x_i) + \cdots$$

This shows that when $f''(x_i) < 0$, the finite difference approximation of the first derivative is less than the true value. This point is also shown graphically in **Figure 3.4a** since $f''(x_i)$ is negative for the curve in this figure. This result also shows that

for a relatively small value of Δx, the error of this forward difference approximation of the first derivative is proportional to Δx. That is, when Δx is small, the coefficients of $f'''(x_i)$ and higher order derivatives will be considerably smaller than the coefficient for $f''(x_i)$; therefore, the error of this approximation is shown to vary directly with Δx. Thus, this finite difference approximation is referred to as an "order Δx approximation."

Likewise, the Taylor series expansion for $f(x_{i-1})$ about $x = x_i$ is

$$f(x_{i-1}) = f(x_i) - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + \cdots$$

Solving for $f'(x)$ yields

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{\Delta x} + \frac{\Delta x}{2} f''(x_i) - \frac{\Delta x^2}{6} f'''(x_i) + \cdots$$

This result is shown in **Figure 3.4b** as the backward difference approximation of the first derivative. This is also an order Δx approximation.

In order to derive the central difference approximation of the first derivative, we must consider the Taylor series expansion for $f(x_{i-1})$ and $f(x_{i+1})$ both about $x = x_i$:

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + \cdots \tag{3.2}$$

$$f(x_{i-1}) = f(x_i) - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + \cdots \tag{3.3}$$

Subtracting these equations yields

$$f(x_{i+1}) - f(x_{i-1}) = 2\Delta x f'(x_i) + \frac{\Delta x^3}{3} f'''(x_i) + \cdots$$

Solving for $f'(x_i)$ yields

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{\Delta x^2}{6} f'''(x_i) + \cdots \tag{3.4}$$

This result is shown in **Figure 3.4c**. Note that the central difference approximation of the first derivative is an order Δx^2 approximation.

Now if we add **Equations 3.2** and **3.3**, the following results:

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + \Delta x^2 f''(x_i) + \frac{\Delta x^4}{12} f''''(x_i) + \cdots$$

Solving for $f''(x_i)$ yields

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2} - \frac{\Delta x^2}{12} f''''(x_i) + \cdots \quad (3.5)$$

This result is the central difference approximation of the second derivative. It is also an order Δx^2 [i.e., $O(\Delta x^2)$] approximation, which is more accurate than an order Δx approximation.

Example 3.2 Application of the Finite Difference Approximations

Problem Statement

Consider the following function:

$$f(x) = e^x$$

Compare the central difference approximations of the first and second derivatives for $\Delta x = 0.5$, 0.1, and 0.01 with the exact value at $x = 1$.

Solution

At $x = 1$ the exact values of the first and second derivatives are

$$f'(x) = e = 2.718282$$

and

$$f''(x) = e = 2.718282$$

Case I

For $\Delta x = 0.5$, $x_{i-1} = 0.5$, $x_i = 1.0$, and $x_{i+1} = 1.5$,

$$f(x_{i-1}) = 1.649$$

$$f(x_i) = 2.718$$

$$f(x_{i+1}) = 4.482$$

Using the central difference formulas for the first and second derivatives yields

$$f'(1.0) = \frac{4.482 - 1.649}{2(0.5)} = 2.833$$

$$f''(1.0) = \frac{4.482 - 2(2.718) + 1.649}{(0.5)^2} = 2.775$$

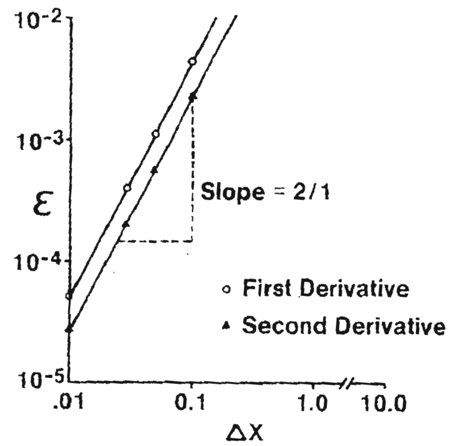

Figure 3.5 Effect of step size on the error of the approximation.

Case II

For $\Delta x = 0.1$, $x_{i-1} = 0.9$, and $x_{i+1} = 1.1$,

$$f'(1.0) = 2.723$$

$$f''(1.0) = 2.721$$

Case III

For $\Delta x = 0.01$, $x_{i-1} = 0.99$, and $x_{i+1} = 1.01$,

$$f'(1.0) = 2.718327$$

$$f''(1.0) = 2.718305$$

It is apparent that as Δx is decreased, the finite difference approximations approach their analytical or exact values.

Now consider how the error between the finite difference approximation and the analytical value changes with step size, Δx. **Figure 3.5** is a log-log plot of ε, where

$$\varepsilon = |\text{finite difference approximation} - e^{1.0}|$$

versus Δx for the order Δx^2 approximation of the first and second derivatives. Note that both lines have a slope of 2, which implies that

$$\varepsilon = K(\Delta x)^2$$

for both approximations, which is consistent with the derived results. For example, if the step size is reduced by a factor of 2, the error of the finite difference approximation is reduced by a factor of 4. The constant K in this relationship will be different for each different approximation. In fact, K is $f'''(1.0)/6$ for the first derivative and $f''''(1.0)/12$ for the second derivative (see **Equations 3.4** and **3.5**).

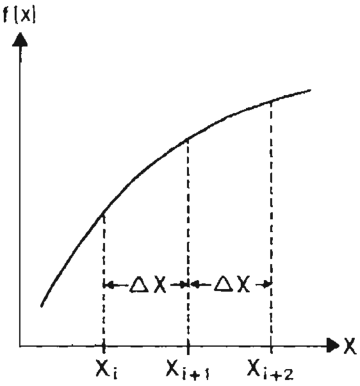

Figure 3.6 Node system for forward difference approximations.

Consider the derivation of a forward difference formula for the node system shown in **Figure 3.6**. As with the derivation of the central difference approximation of the first derivative, we must consider the Taylor series expansion at two points, $f(x_{i+1})$ and $f(x_{i+2})$. Then

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + \cdots$$

$$f(x_{i+2}) = f(x_i) + 2\,\Delta x f'(x_i) + 2\,\Delta x^2 f''(x_i) + \frac{4\Delta x^3}{3} f'''(x_i) + \cdots$$

Eliminating $f''(x_i)$ yields

$$4 f(x_{i+1}) - f(x_{i+2}) = 3 f(x_i) + 2\Delta x f'(x_i) - \frac{2}{3}\Delta x^3 f'''(x_i) + \cdots$$

Solving for $f'(x_i)$ yields

$$f'(x_i) = \frac{-3 f(x_i) + 4 f(x_{i+1}) - f(x_{i+2})}{2\Delta x} + \frac{1}{3}\Delta x^2 f'''(x_i) + \cdots$$

Therefore, this is a forward difference order Δx^2 approximation of the first derivative.

Consider the node arrangement shown in **Figure 3.7**, noting that unequal node spacing is used. The central difference approximation of the first derivative can be determined using the Taylor series expansion for $f(x_{i+1})$ and $f(x_{i-1})$; i.e.,

$$f(x_{i+1}) = f(x_i) + \Delta x_2 f'(x_i) + \frac{\Delta x_2^2}{2} f''(x_i) + \frac{\Delta x_2^3}{6} f'''(x_i) + \cdots$$

$$f(x_{i-1}) = f(x_i) - \Delta x_1 f'(x_i) + \frac{\Delta x_1^2}{2} f''(x_i) - \frac{\Delta x_1^3}{6} f'''(x_i) + \cdots$$

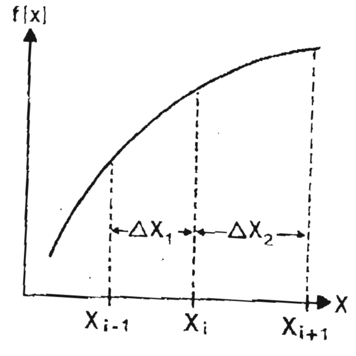

Figure 3.7 Unequal node spacing.

Eliminating $f''(x_i)$ and solving for $f'(x_i)$ yields

$$f'(x_i) = \frac{\Delta x_1^2 f(x_{i+1}) - \Delta x_2^2 f(x_{i-1}) + (\Delta x_2^2 - \Delta x_1^2) f(x_i)}{\Delta x_1 \Delta x_2^2 + \Delta x_2 \Delta x_1^2} - \frac{\Delta x_1 \Delta x_2}{6} f'''(x_i) + \cdots \tag{3.6}$$

Therefore, this finite difference approximation has an error the order of $\Delta x_1 \Delta x_2$. Note that by setting $\Delta x_1 = \Delta x_2$, **Equation 3.6** is found to be equivalent to **Equation 3.4**. In this manner, finite difference approximations can be developed for the case of unequal spacing between node points.

For the case of the central difference approximations, Taylor series expansions were used for two node points other than the base node point (x_i). The result was order Δx^2 approximations. If Taylor series expansions are written for additional nodes, higher order approximations can be derived. But in order to determine exactly what the order of an approximation is, one must retain the error term during the derivation process. **Tables 3.2** and **3.3** list finite difference formulas for order Δx and order Δx^2 approximations. Each table contains forward, backward, and central difference approximations for the first and second derivatives. Finite difference approximations for higher order derivatives and $O(\Delta x^4)$ approximations are tabulated by Chapra and Canale [1].

Section Summary

Taylor series expansions have been used to develop forward, backward, and central difference approximations for the first and second derivatives. These approximations have an error that is of the order of Δx or Δx^2. Using smaller step sizes, Δx, or higher order approximating formulas will result in more accurate approximations.

Table 3.2 Order Δx Approximations for First and Second Derivatives

Forward Difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{\Delta x}$	**(3.7)**
	$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{\Delta x^2}$	**(3.8)**
Backward Difference	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{\Delta x}$	**(3.9)**
	$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{\Delta x^2}$	**(3.10)**
Central Difference	None	

Table 3.3 Order Δx^2 Approximations for First and Second Derivatives

Forward Difference	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2\Delta x}$	**(3.11)**
	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{\Delta x^2}$	**(3.12)**
Backward Difference	$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2\Delta x}$	**(3.13)**
	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{\Delta x^2}$	**(3.14)**
Central Difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}$	**(3.15)**
	$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2}$	**(3.16)**