Numerical Differentiation and Integration

Objectives

- Knowing how to implement Finite Difference Methods for evaluating the derivative of function and discrete data.
- Know how to implement Trapezoidal Rule and Simpson's 1/3 Rule to integrate function and discrete data.

Finite Differences for Numerical Differentiation

In engineering and scientific problems, sometime we need to solve for the derivative of complex functions or discrete data. Using analytical method may be troublesome for these cases. Finite difference is one of useful numerical techniques that we can use for evaluating the derivatives. This technique starts from Taylor's Series expansion which is given by

$$f(x_{j+1}) = f(x_j) + (x_{j+1} - x_j)f'(x_j) + \frac{(x_{j+1} - x_j)^2}{2!} f''(x_j) + \cdots + \frac{(x_{j+1} - x_j)^n}{n!} f^n(x_j) \quad (1)$$

Then we can rearrange Eq. (1) to estimate $f'(x_j)$ as

$$(x_{j+1} - x_j)f'(x_j) = f(x_{j+1}) - f(x_j) - \frac{(x_{j+1} - x_j)^2}{2!} f''(x_j) + \cdots + \frac{(x_{j+1} - x_j)^n}{n!} f^n(x_j) \quad (2)$$

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{x_{j+1} - x_j} - \frac{(x_{j+1} - x_j)}{2!} f''(x_j) + \cdots + \frac{(x_{j+1} - x_j)^{n-1}}{n!} f^n(x_j) \quad (3)$$

Let $(x_{j+1} - x_j) = h$ which is step size for estimation.

And $O(h) = -\frac{(x_{j+1} - x_j)}{2!} f''(x_j) + \cdots + \frac{(x_{j+1} - x_j)^{n-1}}{n!} f^n(x_j)$ which is prescribed as leading error or truncation error. This error is a function of the step size, *h*.

Thus, we obtain

$$f'(x_j) = \frac{f(x_{j+1}) \; - \; f(x_j)}{h} \; + O(h) \qquad (4)$$

This estimation is called **Forward Difference.**

We can also estimate the derivatives from the following form of Taylor's Series expansion.

$$f(x_{j-1}) = f(x_j) - (x_{j-1} - x_j) f'(x_j) + \frac{(x_{j-1} - x_j)^2}{2!} f''(x_j) + \cdots + \frac{(x_{j-1} - x_j)^n}{n!} f^n(x_j) \qquad (5)$$

We also need to obtain, then we have

$$f'(x_{j-1}) = \frac{f(x_j) - f'(x_{j-1})}{x_{j-1} - x_j} + \frac{(x_{j-1} - x_j)}{2!} f''(x_j) + \cdots + \frac{(x_{j-1} - x_j)^{n-1}}{n!} f^n(x_j) \qquad (6)$$

Again let $(x_{j-1} - x_j) = h$ which is step size for estimation.

And $O(h) = \dfrac{(x_{j-1} - x_j)}{2!} f''(x_j) + \cdots + \dfrac{(x_{j-1} - x_j)^{n-1}}{n!} f^n(x_j)$ which is prescribed as leading error or truncation error. This error is a function of the step size, *h*.

Thus, we have

$$f'(x_j) = \frac{f(x_j) \; - \; f(x_{j-1})}{h} \; + O(h) \qquad (7)$$

This estimation is called **Backward Difference**.

If we rewrite Eq. (1) and Eq. (5), we have

$$f(x_{j+1}) = f(x_j) \; + \; hf'(x_j) \; + \; \frac{h^2}{2!} f''(x_j) \; + \; \frac{h3}{3!} f'''(x_j) \; + \cdots + \; \frac{h^n}{n!} f^n(x_j) \qquad (8)$$

$$f(x_{j-1}) = f(x_j) \; - \; hf'(x_j) \; + \; \frac{h^2}{2!} f''(x_j) \; - \; \frac{h3}{3!} f'''(x_j) \; + \cdots + \; \frac{h^n}{n!} f^n(x_j) \qquad (9)$$

The subtraction of Eq. (9) from Eq. (9), Eq. (8) – Eq. (9), generates

$$f'(x_j) = \frac{f(x_{j+1}) \quad - \quad f(x_{j-1})}{2h} \quad + \quad \frac{h^2}{2!} f'''(x_j) \quad + \cdots$$

Or

$$f'(x_j) = \frac{f(x_{j+1}) \quad - \quad f(x_{j-1})}{2h} \quad + \quad O(h^2) \tag{10}$$

This estimation is called **Central Difference**.

Now, if we sum Eq. (8) and Eq. (9), then we can estimate the second derivatives as follows:

$$f''(x_j) = \frac{f(x_{j+1}) \quad -2f(x_j) \quad f(x_{j-1})}{h^2} \quad + \quad O(h^2) \tag{11}$$

This is also called **Central Difference for the second derivative**.

Example 1 Find the acceleration from the following data.

t (hr)	0	2	4	6	8
v (km/hr)	0	10	80	60	70

Where t = time (hr)

v = velocity (m/s)

1.1 Use Forward Difference to find the acceleration.

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1.2 Use Backward Difference to find the acceleration.

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1.3 Use Central Difference to find the acceleration.

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Example 2 Find $f'(0.1)$ and $f''(0.1)$ for $f(x) = xe^{1-x^2}$.

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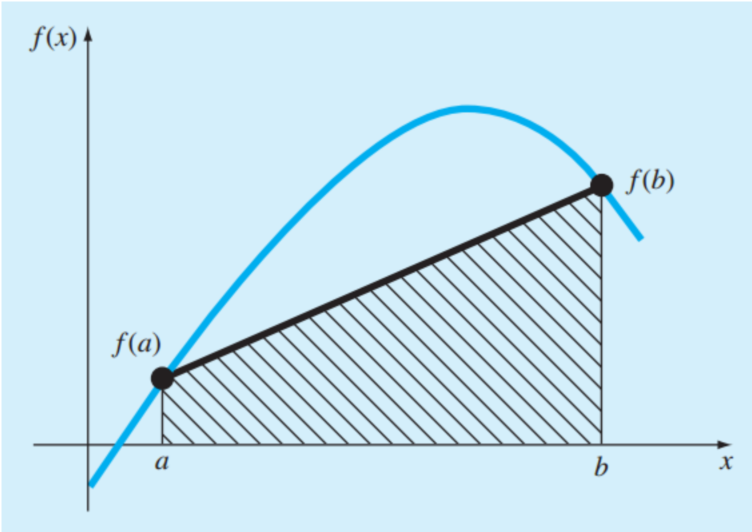
Numerical Integration

1. **Trapezoidal Rule**

The concept of this technique is equivalent to the area approximation of the curve. The area under the curve is approximated by the trapezoid. The point on the curve is connected by the straight line as follows:



If we have the function f(x) which is a linear function, the integral from a to b for f(x) is

$$I = \int_a^b f(x)dx \tag{12}$$

Where f(x) is obtained by linear interpolation. Then

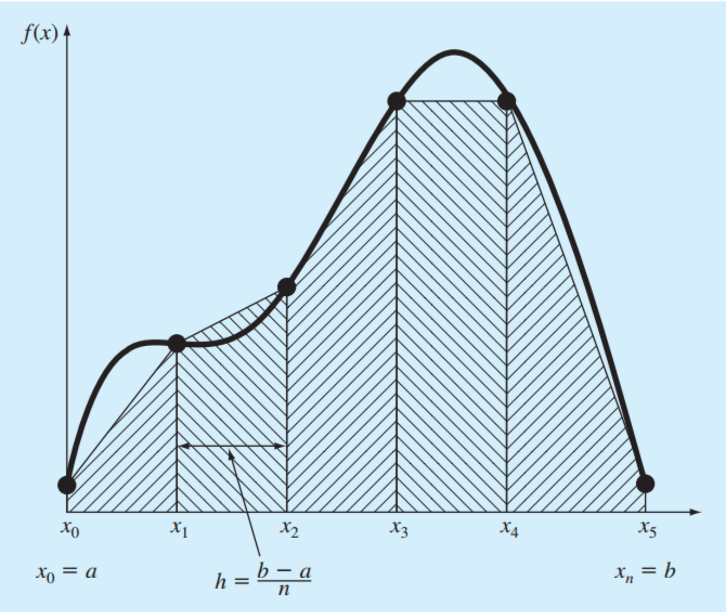
$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b-a}(x-a) \right] dx \tag{13}$$

The result of the integration is

$$I = (b-a)\frac{f(a)+f(b)}{2} \tag{14}$$

The composite Trapezoidal Rule

To improve the accuracy of the trapezoidal rule, the integration interval from a to b is split into several segments. The area is split into a number of trapezoids. Thus, the entire area is obtained by the summation of the area of individual trapezoids.



If the integration interval (from *a* to *b*) is divided into *n* segments of equal width, the width of an individual segment is given by

$$h = \frac{b-a}{n} \tag{15}$$

If *a* and *b* are designed as x_0 and x_n, respectively, the total integral can be represented as

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx \tag{16}$$

Substituting the trapezoidal rule for each integral yields

$$I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2} \tag{17}$$

Eq. (17) can be rewritten as

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right] \tag{18}$$

Example 3 Use the three-segment trapezoidal rule to estimate the integral of

$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4$ from a = 0 to b =0.6.

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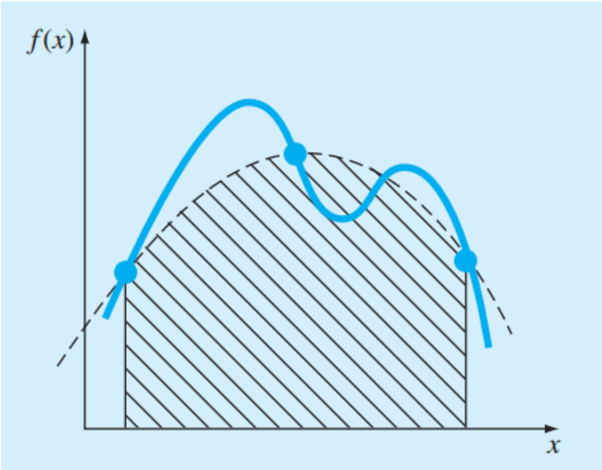
2. **Simpson's 1/3 Rule**

Simpson's 1/3 rule corresponds to the case where the second-order polynomial is implemented to connect the point on the curve. The area under the curve is equivalent to the area under the parabola as follows:



The integral yields

$$I = \int_a^b f(x)dx$$

$$= \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_1)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] \quad (19)$$

Where *a* and *b* are designated as x_0 and x_2, respectively. The results of the integration is

$$I = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \quad (20)$$

The composite Simpson's 1/3 rule

The accuracy of the Simpson's 1/3 rule can be improved by dividing the integration interval into a number of segments of equal width. The total integral can be represented as

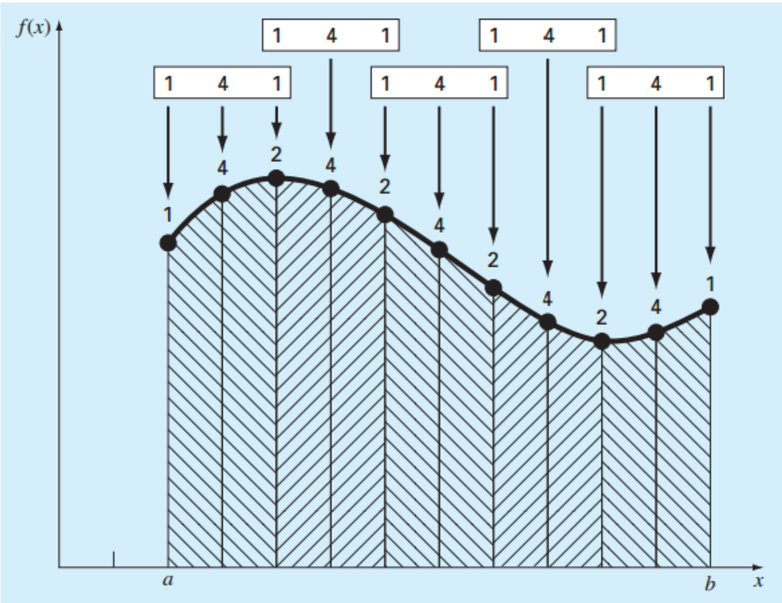
$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

Substituting Simpson's 1/3 rule for each integral yields

$$I = 2h\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6} \qquad (21)$$

Eq. (21) can be written grouping terms as follows:

$$I = (b-a)\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i)+2\sum_{j=2,4,6}^{n-2} f(x_j)+f(x_n)}{3n} \qquad (22)$$



Example 4 Use the composite Simpson's 1/3 rule to estimate the integral of

$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4$ from a = 0 to b =0.8, where n=4.

Exercises

1. The following data were collected for the distance travel versus time for a rocket:

t [s]	0	25	50	75	100	125
y [km]	0	32	58	78	92	100

   a) Use forward difference to estimate the rocket's velocity at t = 50 s.

   b) Use backward difference to estimate the rocket's velocity at t = 50 s.

   c) Use central difference to estimate the rocket's velocity at t = 100 s.

   d) Use forward difference to estimate the rocket's acceleration at t = 100 s.

2. Evaluate the following integral:

$$\int_{-2}^{4}(1-x-4x^3+2x^5)dx$$

   a) Use analytical method.

   b) Use composite Trapezoidal rule with n = 4.

   c) Use composite simpson's 1/3 rule with n = 4.

3. From the following data, evaluate the integral from a = 0 to b = 1.2 using **a)** analytical methods, **b)** a composite trapezoidal rule with n = 2, **c)** composite simpson's 1/3 rule with n = 3.

x	0	0.1	0.3	0.5	0.7	0.95	1.2
f(x)	1	0.9048	0.7408	0.6065	0.4966	0.3867	0.3012