Chapter 04-Numerical Differentiation and Integration

Lecturer- Ms.M.W.S. Randunu

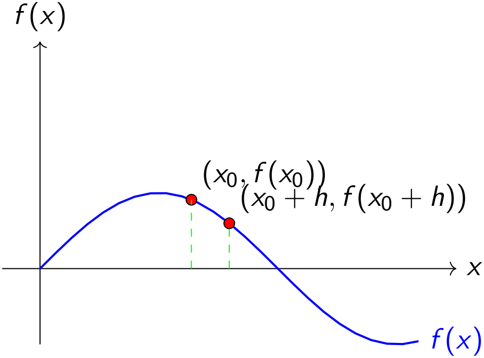
Department of Interdisiplinary Studies,University of Ruhuna.

Numerical differentiation is used to estimate the derivative of a function at a given point, while numerical integration seeks to approximate the area under a curve, providing insights into the behavior of functions over intervals. In this chapter, we will explore

the foundational concepts of numerical differentiation and integration, discuss common methods and examine practical examples that illustrate the applicability of these techniques in real-world scenarios.

Suppose we have a function $f(x)$ which is differentiable at a point $x = x_0$. The derivative of f at x_0 is given by:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$



To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$ and that $x_1 = x_0 + h$ for some $h \neq 0$, that is sufficiently small to ensure that $x_1 \in [a, b]$.
We construct the first Lagrange polynomial $P_{0,1}(x)$ for f determined by x_0 and x_1, with its error term,

$$
\begin{aligned}
f(x) &= P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\
&= f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0} + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\
&= f(x_0)\frac{(x-x_0-h)}{-h} + f(x_0+h)\frac{(x-x_0)}{h} + \frac{(x-x_0)(x-x_0-h)}{2!} f''
\end{aligned}
$$

for some $\xi(x) \in [a, b]$.

Differentiating gives,

$$\begin{aligned}
f'(x) &= \frac{f(x_0)}{-h} + \frac{f(x_0+h)}{h} + D_x \frac{(x-x_0)(x-x_0-h)}{2!} f''(\xi(x)) \\
&= \frac{f(x_0+h)-f(x_0)}{h} + D_x \frac{(x-x_0)(x-x_0-h)}{2!} f''(\xi(x)) \\
&= \frac{f(x_0+h)-f(x_0)}{h} + [\frac{(x-x_0)+(x-x_0-h)}{2}] f''(\xi(x)) + \frac{(x-x_0}{} \\
&= \frac{f(x_0+h)-f(x_0)}{h} + [\frac{2(x-x_0)-h}{2}] f''(\xi(x)) + \frac{(x-x_0)(x-x_0}{2}
\end{aligned}$$

So

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$.Then the error cannot be estimated.
When $x = x_0$, coefficient of $D_x f''(\xi(x))$ is 0 , and formula simplifies to,

$$f'(x) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

For small values of h, the difference quotient $\frac{f(x_0+h)-f(x_0)}{h}$ can be used to approximate $f'(x)$ with an error bounded on $\frac{M|h|}{2}$, where M is a bound on $|f''(x)|$ for $x \in [a, b]$.

This formula is known as,

- Forward difference formula if $h > 0$.

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h}$$

- Backward difference formula if $h < 0$

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h}$$

To obtain general derivative approximation formula, Suppose that $x_0, x_1, ..., x_n$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$.

Then we can write

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)(x-x_1)...(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

for some $\xi(x) \in I$, where $L_k(x)$ denotes the k^{th} Langrage coefficient polynomial for f at $x_0, x_1, x_2, ...x_n$. Differentiating this expression gives,

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k^{'}(x) + D_x[\frac{(x-x_0)(x-x_1)...(x-x_n)}{(n+1)!}]f^{(n+1)}(\xi(x)) +$$

Hence, if x is one of the numbers x_j, the term multiplying $D_x[f^{(n+1)}(\xi(x))]$ is 0 and the formula become

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k^{'}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{k=0,k\neq j}^{n} (x_j - x_k) \qquad (1)$$

Which is called a $(n+1)$-point formula to approximate $f^{'(x_j)}$. In general, using more evaluation points in the above equation produces greater accuracy. The most common formulas are those involving three and five evaluation points. Now we derive the useful three-point formula. since

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

we have

$$L_0^{'}(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

Similarly

$$L_1^{'}(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$
$$L_2^{'}(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

Hence by using equation 4.1 ,

$$f'(x_j) = f(x_0)L_0^{'}(x_j) + f(x_1)L_1^{'}(x_j) + f(x_2)L_2^{'}(x_j) + \frac{f^3(\xi(x_j))}{3!} \prod_{k=0,k\neq j}^{2} (x_j -$$

$$f'(x_j) = f(x_0)[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}] + f(x_1)\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{2x_j}{(x_2 -} \quad (2)$$

for each $j = 0, 1, 2, ...$ where the notation ξ_j indicates that this point depends on x_j.

The three formulas from equation 4.2 become especially useful if the nodes are equally spaced, that is, when $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ for some $h \neq 0$.
We will assume equally spaced nodes through the rest of this section.
Using equation 4.2 with $x_j = x_0, x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ gives,

$$f'(x_0) = \frac{1}{h}[\frac{-3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

Doing the same for $x_j = x_1$ gives

$$f'(x_1) = \frac{1}{h}[\frac{-1}{2}f(x_0) + \frac{1}{2}f(x_2)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

and for $x_j = x_2$

$$f'(x_2) = \frac{1}{h}[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)] - \frac{h^2}{3}f^{(3)}(\xi_2)$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as,

$$f'(x_0) = \frac{1}{h}[\frac{-3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$
$$f'(x_0+h) = \frac{1}{h}[\frac{-1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$
$$f'(x_0+2h) = \frac{1}{h}[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)] - \frac{h^2}{3}f^{(3)}(\xi_2)$$

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation for $f^{'(x_0)}$.A similar change x_0 for $x_0 + 2h$is used in the last equation .This gives three formulas for approximating $f^{'(x_0)}$:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$
$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$
$$f'(x_0) = \frac{1}{2h}[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] - \frac{h^2}{3}f^{(3)}(\xi_2)$$

Finally, note that since the last of these equations can be obtained from the first by simply replacing h with $-h$, Hence are actually two formulas.

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\xi_0)$$

(3)

Where ξ_0 lies between x_0 and $x_0 + 2h$.

$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

(4)

Where ξ_1 lies between $(x_0 - h)$ and $(x_0 + h)$.

Example 1: Use the forward-difference and backward difference formulas to determine each missing entry in the following table.

x	$f(x)$
0.5	0.4794
0.6	0.5646
0.7	0.6442

Example 2: Value for $f(x) = xe^x$ are given in the following table.

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.1489577
2.2	19.855030

Since $f'(x) = (x+1)e^x$, we have $f^{'(2.0)=22.167168}$.
Approximating $f^{'(2.0)}$ using the various three-point formulas produces the following results.
Using 4.3 with $h = 0.1, x_0 = 2.0$

$$\begin{aligned} f^{'(2.0)} &= \frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2)] \\ &= 22.032310 \end{aligned}$$

Using 4.3 with $h = -0.1, x_0 = 2.0$

$$\begin{aligned} f^{'(2.0)} &= \frac{-1}{0.2}[-3f(2.0) + 4f(1.9) - f(1.8)] \\ &= 22.054525 \end{aligned}$$

Using 4.4 with $h = 0.1, x_0 = 2.0$

$$\begin{aligned} f^{'(2.0)} &= \frac{1}{0.2}[f(2.2) - f(1.8)] \\ &= 22.228790 \end{aligned}$$

with $h = 0.2, x_0 = 2.0$

$$\begin{aligned} f^{'(2.0)} &= \frac{1}{4}[f(2.2) - f(1.8)] \\ &= 22.414163 \end{aligned}$$

Numerical integration is a collection of algorithms for calculating the approximate value of integrals when an analytical solution is difficult or impossible to obtain. This is particularly useful for functions that are complex or for data sets.

Integration is fundamentally defined as the process of calculating the area under a curve represented by a function $f(x)$ over a specified interval $[a, b]$. Mathematically, this is expressed as:

$$\int_a^b f(x)\,dx$$

This integral gives the total area between the curve $f(x)$, the x-axis, and the vertical lines $x = a$ and $x = b$.
Integration not only provides a way to find areas but also connects various fields through its applications in solving real-world problems.

The need often arises for evaluating the definite integral of a function that has no explicit anti derivatives or whose anti derivatives is not easy to obtain. The basic method involved in approximating

$$\int_a^b f(x)\,dx$$

is called numerical quadrature. It uses a sum

$$\sum_{i=0}^{n} a_i f(x_i)$$

to approximate

$$\int_a^b f(x)\,dx$$

The methods of quadrature in this section are based on the interpolation polynomials.We first select a set of distinct nodes $x_0, x_1, ..x_n$ from the interval $[a, b]$.
Then we integrate the Lagrange interpolating polynomial,

$$P_n(x) = \sum_{i=0}^{n} f(x_i)L(x_i)$$

and the truncation error term over [a,b],

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)L(x_i)\,dx + \int_a^b \prod_{i=0}^{n}(x-x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx$$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i)\,dx + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x-x_i)f^{(n+1)}(\xi(x))\,dx$$

Where $\xi(x)$is an $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)\, dx$$

, for each $i = 0, 1, 2, ..., n$. The quadrature formula is, therefore,

$$\int_a^b f(x)\, dx \approx \sum_{i=0}^{n} a_i f(x_i)\, dx$$

with error given by,

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x))\, dx$$

Let's consider formulas produced by using 1st Lagrange polynomials with equally space nodes. This gives the Trapezoidal Rule, Which is commonly introduced in calculus courses.

lso we can obtain the "Simpson's rule" by using second Lagrange polynomial with equally spaced nodes.
To derive the Trapezoidal rule for approximating

$$\int_a^b f(x)\,dx$$

, Let $x_0 = a, x_1 = b, h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} [\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)]\,dx + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))($$

Since $(x - x_0)(x - x_1)$ doesn't change sign on $[x_0, x_1]$, the weighted mean value theorem for integrals can be applied to the error term to give, for some $\xi \in (x_0, x_1)$.

$$\frac{1}{2}\int_{x_0}^{x_1} f^{''}(\xi(x))(x-x_0)(x-x_1)\,dx = \frac{1}{2}f^{''}(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx$$

$$\frac{1}{2}\int_{x_0}^{x_1} f^{''}(\xi(x))(x-x_0)(x-x_1)\,dx = \frac{-h^3}{6}f^{''}(\xi)$$

So

$$\int_a^b f(x)\,dx = [\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)]_{x_0}^{x_1}\,dx - \frac{h^3}{6}f^{''}(\xi)$$

$$\int_a^b f(x)\,dx = \frac{(x_1-x_0)}{2}[f(x_0)+f(x_1)] - \frac{h^3}{6}f^{''}(\xi)$$

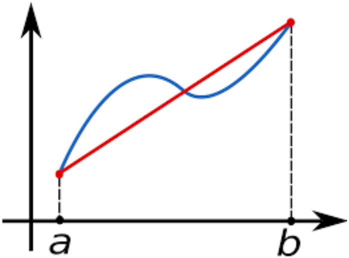
since $h = x_1 - x_0$, We have the following rule:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left(f(x_0)+f(x_1)\right) - \frac{h^3}{6}f^{''}(\xi)$$

This is called the Trapezoidal rule because when f is a function with positive values

$$\int_a^b f(x)\,dx$$

is approximated by the area in a trapezoid, as shown in below:



The Trapezoidal Rule is a numerical method used to approximate the definite integral of a function. It works by dividing the area under the curve into trapezoids rather than rectangles, leading to a better approximation.

For a continuous function $f(x)$ over the interval $[a, b]$, the Trapezoidal Rule is expressed as:

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{2}\left(f(a) + f(b)\right)$$

If the interval is subdivided into n equal segments of width $h = \frac{b-a}{n}$, the formula becomes:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right)$$

where $x_i = a + ih$ for $i = 0, 1, \ldots, n$.

The error for the Trapezoidal Rule is given by:

$$E_T = -\frac{(b-a)^3}{12n^2} f''(\xi)$$

for some $\xi \in (a, b)$. This indicates that the error decreases quadratically as the number of subdivisions increases.

Example 1: The Trapezoidal rul for a function f on the interval$[0, 2]$ is,

$$\int_0^2 f(x)\, dx \approx f(0) + f(2)$$

Example 2: Approximate the following integrals using the Trapezoidal rule,

1. $\int_{0.5}^{1} x^4\, dx$
2. $\int_{0}^{0.5} \frac{2}{x-4}\, dx$
3. $\int_{1}^{1.5} x^2 lnx\, dx$
4. $\int_{0}^{1} x^2 e^{-x}\, dx$

Example 3:
Consider the function $f(x) = \sin(x)$ over the interval $[0, \pi]$. We will use the Trapezoidal Rule to approximate the integral

$$\int_0^\pi \sin(x)\, dx.$$

Gaussian Quadrature chooses the points for evaluation in an optimal, rather than equally spaced way. The nodes $x_0, x_1, ..., x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, ..., c_n$ are chosen to minimize the expected error obtained in the approximation,

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

To measure this accuracy, we assume that the best choice of these values is that which produces the exact results for the largest class of polynomials.[ie., the choice that gives the greatest precision]

The coefficients $c_1, c_2, ..., c_n$ in the approximation formula are arbitrary and the nodes $x_0, x_1, ..., x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration.

This gives us $2n$ parameters to choose.If the coefficients of a polynomial are considered parameters the class of polynomials of degree at most $2n - 1$ also contain $2n$ parameters. This is the largest class of polynomials for which it is reasonable to expect the formula to be exact.

To illustrate the procedure for choosing the appropriate parameters, We consider how to select the coefficients and nodes when $n = 2$ and interval of integration is $[-1, 1]$.

Then we discuss the more general situation for an arbitrary choice of nodes and coefficients and consider how the technique is modified when integrating over an arbitrary interval.

Suppose we want to determine c_1, c_2, x_1 and x_2 so that the integration formula,

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact results whenever $f(x)$ is a polynomial of degree $2n - 1 = 2(2) - 1 = 3$ or less, that is when,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

, for some collection of constraints a_0, a_1, a_2 and a_3.

Because

$$\int (a_0+a_1x+a_2x^2+a_3x^3)\,dx = a_0\int 1\,dx+a_1\int x\,dx+a_2\int x^2\,dx+a_3\int x^3$$

this is equivalent to showing that the formula gives exact results when $f(x)$ is $1, x, x^2, x^3$.Hence we $c_1 c_2, x_1$ and x_2 so that

$$c_1 + c_2 = \int_{-1}^{1} 1\,dx = 2$$

$$c_1x_1 + c_2x_2 = \int_{-1}^{1} x\,dx = 0$$

$$c_1x_1^2 + c_2x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}$$

$$c_1x_1^3 + c_2x_2^3 = \int_{-1}^{1} x^3\,dx = 0$$

So it shows that this system of equations has the unique solution,

$$c_1 = 1, c_2 = 1, x_1 = \frac{-\sqrt{3}}{3}, x_2 = \frac{\sqrt{3}}{3}$$

Similarly we can find nodes and coefficients for higher degree polynomials giving exact results results. These coefficients can be found using Legendre polynomials as well. Transformation of the interval $[-1, 1]$ to $[a, b]$:
The linear transformation

$$t = [\frac{1}{(b-a)}(2x - a - b)]$$

$$x = \frac{1}{2}[(b-a)t + a + b]$$

translate the interval $[a, b]$ to $[-1, 1]$. Hence,

$$\int_a^b f(x)\, dx = \int_{-1}^{1} f(\frac{1}{2}[(b-a)t + a + b])\frac{(b-a)}{2}\, dt$$

Example 1: Consider the problem of finding approximations to

$$\int_1^{1.5} e^{-x^2}\,dx$$

when $n = 2$.

$$\begin{aligned}
\int_{1}^{1.5} e^{-x^2}\,dx &= \int_{-1}^{1} f[\frac{(b-a)t+a+b}{2}]\frac{(b-a)}{2}\,dt \\
&= \int_{-1}^{1} f[\frac{(1.5-1)t+1.5+1}{2}]\frac{(1.5-1)}{2}\,dt \\
&= 0.25\int_{-1}^{1} f[\frac{0.5t+2.5}{2}]\,dt \\
&= \frac{1}{4}\int_{-1}^{1} e^{-[\frac{(t+5)^2}{16}]}\,dt \\
&\approx \frac{1}{4}[f(-\frac{\sqrt{3}}{3})+f(\frac{\sqrt{3}}{3})] \\
&= \frac{1}{4}[f(-0.577350269)+f(0.577350269)] \\
&= \frac{1}{4}[e^{-\frac{(-0.577350269)^2}{16}}+e^{-\frac{(0.577350269)^2}{16}}] \\
&= 0.1094003
\end{aligned}$$

Example 2: Approximate the following integrals using Gaussian quadrature with $n = 2$

1. $\int_1^{1.5} x^2 lnx \, dx$
2. $\int_0^1 x^2 e^{-x} \, dx$

For $n = 2$:

- Points: $x_1 = -\frac{1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}}$
- Weights: $c_1 = c_2 = 1$

For $n = 3$:

- Points: $x_1 = -\sqrt{\frac{3}{5}}, \quad x_2 = 0, \quad x_3 = \sqrt{\frac{3}{5}}$
- Weights: $c_1 = c_3 = \frac{5}{9}, \quad c_2 = \frac{8}{9}$

Example 3:
Consider the function $f(x) = e^x$ over the interval $[0, 1]$. We will use Gaussian Quadrature with $n = 2$ to approximate the integral

$$\int_0^1 e^x \, dx.$$

Gaussian Quadrature achieves high accuracy with fewer points compared to other methods. The error depends on the degree of the polynomial being integrated and is significantly smaller than that of simpler methods like the Trapezoidal Rule.

- **High Precision Requirements**: Particularly useful in physics and engineering when dealing with high-degree polynomials.
- **Complex Integrals**: Effective for functions that are not easily handled by traditional methods.

If B is our estimate of some quantity with an actual value of A, then the absolute error is given by:

$$\text{Absolute Error} = |A - B|$$

The relative error, expressed as a percentage of the actual value, is given by:

$$\text{Relative Error} = \left|\frac{A - B}{A}\right| \times 100\%$$