

Sect.1 Numerical Differentiation

Numerical differentiation usually arises in one of the two primary contexts. At the first places, the objective is to approximate the value of a derivative of a function defined by a discrete set of data points. In the second context, the aim is to drive an analytic expression which approximate derivatives through linear combination of function values.

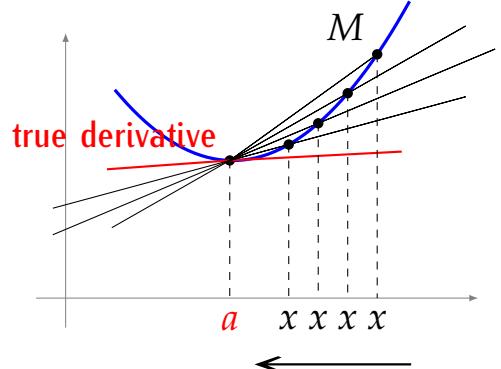
Given a set of discrete data points, two principal approaches can be employed to calculate a numerical approximation of the derivative at a specific point x_i . The first approach is to use a finite difference approximation for the derivative. A finite difference approximation of a derivative at a point x_i is an approximate calculation based on the value of points in the neighborhood of x_i . The second approach is to approximate the points with an analytical expression that can be easily differentiated, and then to calculate the derivative by differentiating the analytical expression.

Sect.2 Finite difference approximation of the derivative

The derivative $f'(x)$ of a function f at a point $x = a$ is defined by

$$\frac{df(x)}{dx} \Big|_{x=a} = f'(a) = \lim_{x \rightarrow a} \frac{f(x) - f(a)}{x - a}$$

As illustrated graphically, the derivative is the value of the slope of the tangent line to the function at $x = a$. The derivative represents the slope of the tangent line to the function at the point $x = a$. It is computed by considering a neighboring point x near a and determining the slope of the secant line connecting these two points.

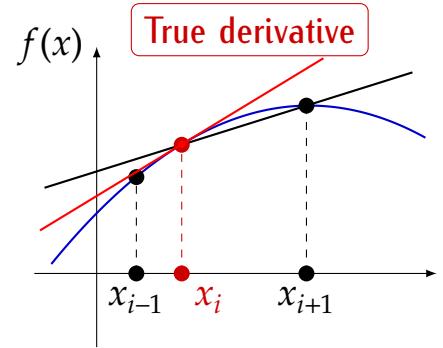


Forward, backward, and central difference formulas for the first derivative

The forward, backward, and central finite difference formulas are the simplest finite difference approximations of the derivative. In these approximations, the derivative at point x_i is calculated from the values of two points. The derivative is estimated as the value of the slope of the line that connects the two points.

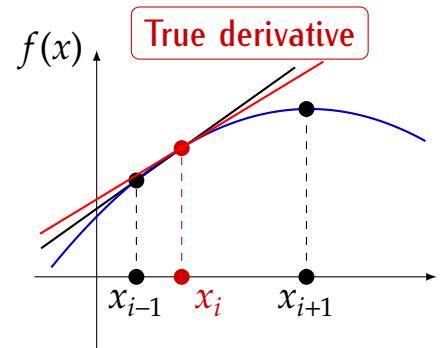
Forward Finite Difference: is the slope of the line that connects points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$

$$\frac{df(x)}{dx} \Big|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$



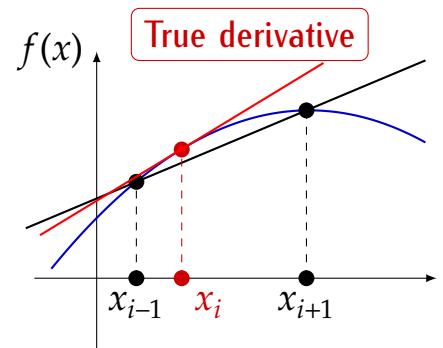
Backward Finite Difference: is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_i, f(x_i))$

$$\frac{df(x)}{dx} \Big|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$



Central Finite Difference: is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_{i+1}, f(x_{i+1}))$

$$\frac{df(x)}{dx} \Big|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



The black line represents the approximated derivative.

Sect.3 Finite difference formulas using Taylor series expansion

The forward, backward, and central difference formulas, along with other finite difference approximations for derivatives, can be derived through Taylor series expansions.

Sect.3.1 Finite Difference Formulas of First Derivative

The Taylor series expansion facilitates the derivation of various numerical approximations for the first derivative at a point x_i by using function values at neighboring points.

Two-point forward difference formula for first derivative The value of a function at point x_{i+1} can be approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \quad (1)$$

where $h = x_{i+1} - x_i$ is the spacing between the points. By using two-term Taylor series expansion with a remainder, (1) can be rewritten as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \quad (2)$$

where ξ is a value of x between x_i and x_{i+1} . Solving (2) for $f'(x_i)$ yields

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} - \frac{f''(\xi)}{2!}h. \quad (3)$$

An approximate value of the derivative $f'(x_i)$ can now be calculated by ignoring the second term on the right hand side of (3), which introduces a truncation error on the order of h (written as $O(h)$)

$$\text{truncation error} = \frac{f''(\xi)}{2!}h = O(h)$$

In this case, using the latter notation, the approximated value of the first derivative would be

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \quad (4)$$

Notice that the approximation in (4) is the same as the forward difference formula derived from the above graph.

Two-point backward difference formula for first derivative The backward difference formula can also be derived by application of Taylor series expansion. The value of the function at point x_{i-1} is approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \quad (5)$$

where $h = x_i - x_{i-1}$. By using a two-term Taylor series expansion with a remainder, (5) can be rewritten as

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 \quad (6)$$

where ξ is a value of x between x_{i-1} and x_i . Solving (6) for $f'(x_i)$ yields

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} + \frac{f''(\xi)}{2!}h. \quad (7)$$

An approximate value of the derivative, $f'(x_i)$ can be calculated if the second term on the right-hand side of (7) is ignored. This yields

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \quad (8)$$

which is the same as the backward difference formula obtained graphically before.

Two-point central difference formula for first derivative The central difference formula can be derived by using three terms in the Taylor series expansion and a remainder. The value of the function at point x_{i+1} in terms of the value of the function and its derivatives at point x_i is given by

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \quad (9)$$

where ξ_1 is a value of x between x_i and x_{i+1} . The value of the function at point x_{i-1} in terms of the value of the function and its derivatives at point x_i is given by

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(\xi_2)}{3!}h^3 \quad (10)$$

where ξ_2 is a value of x between x_i and x_{i-1} . In the last two equations, the spacing of the intervals is taken to be equal so that $h = x_{i+1} - x_i = x_i - x_{i-1}$. Subtracting (10) from (9) gives

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3 \quad (11)$$

An estimate for the first derivative is obtained by solving (11) for $f'(x_i)$ while neglecting the remainder terms, which introduces a truncation error of the order of h^2

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \quad (12)$$

The latter approximation is the same as the central difference formula obtained graphically for equally spaced intervals.

An analysis of (4), (8), and (12) reveals that the truncation error in the forward and backward difference approximations is of order h , whereas in the central difference approximation, it is of order h^2 . This demonstrates that the central difference method provides a more precise estimation of the derivative. This improvement in accuracy is illustrated schematically in the geometric interpretation of the central difference where the slope derived from the central difference approximation aligns more closely with the tangent line's slope compared to those obtained from the forward and backward difference methods.

Three-point forward and backward difference formulas for the first derivative

The forward difference formula computes the derivative at a point x_i using the function values at x_i and the subsequent point x_{i+1} . Conversely, the backward difference formula estimates the derivative at x_i by incorporating the values at x_i and the preceding point x_{i-1} . Therefore, the forward difference method is particularly suitable for approximating the first derivative at the initial point x_1 and all interior points, whereas the backward difference approach is applicable at the final point x_n as well as the interior points. In contrast, the central difference formula calculates the first derivative at x_i by utilizing the adjacent points x_{i-1} and x_{i+1} . As a result, for a discretely defined function with n data points, the central difference approximation is only applicable to interior points and cannot be directly employed at the endpoints x_1 or x_n .

The three-point forward difference formula approximates the derivative at a given point x_i using the function values at x_i and the two subsequent points, x_{i+1} and x_{i+2} . This method assumes uniform spacing between points, such that $h = x_{i+2} - x_{i+1} = x_{i+1} - x_i$. The derivation of this formula begins by expressing the function values at x_{i+1} and x_{i+2} in terms of the Taylor series expansion about x_i , retaining up to three terms along with the corresponding remainder

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{f''(x_i)}{2}h^2 + \frac{f'''(\xi_1)}{6}h^3, \quad \xi_1 \in]x_i, x_{i+1}[, \quad (13)$$

$$f(x_{i+2}) = f(x_i) + 2hf'(x_i) + \frac{f''(x_i)}{2}(2h)^2 + \frac{f'''(\xi_2)}{6}(2h)^3, \quad \xi_2 \in]x_i, x_{i+2}[. \quad (14)$$

The latter equations are next combined such that the terms with the second derivative vanish to obtain

$$4f(x_{i+1}) - f(x_{i+2}) = 3f(x_i) + 2f'(x_i)h + \frac{4f'''(\xi_1)}{3!}h^3 + \frac{4f'''(\xi_2)}{3!}(2h)^3 \quad (15)$$

An estimate for the first derivative is obtained by solving (15) for $f'(x_i)$ while neglecting the remainder terms, which introduces a truncation error of the order of h^2

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} + O(h^2). \quad (16)$$

Equation (16) is the three-point forward difference formula that estimates the first derivative at point x_i from the value of the function at that point and at the next two points x_{i+1} and x_{i+2} , with an error of $O(h^2)$. The formula can be used for calculating the derivative at the first point of a function given by a discrete set of n points.

The three-point backward difference formula yields the derivative at point x_i from the value of the function at that point and at the previous two points, x_{i-1} and x_{i-2} . The formula is derived in the

same way that (16) was derived. The three-term Taylor series expansion with a remainder is written for the value of the function at point x_{i-1} , and at point x_{i-2} in terms of the value of the function and its derivatives at point x_i . The equations are then manipulated to obtain an equation without the second derivative terms, which is then solved for $f'(x_i)$. The formula that is obtained is

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2) \quad (17)$$

where $h = x_i - x_{i-1} = x_{i-1} - x_{i-2}$ is the distance between the points.

Sect.3.2 Finite Difference Formulas for the Second Derivative

The same approach used to develop finite difference formulas for the first derivative can be used to develop expressions for higher-order derivatives.

Three-point forward difference formulas for the second derivative at point x_i from the value of that point and the next two points, x_{i+1} and x_{i+2} , is developed by multiplying (13) by 2 and subtracting it from (14). The resulting equation is then solved for $f''(x_i)$

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2} + O(h). \quad (18)$$

Three-point backward difference formulas for the second derivative at point x_i from the value of that point and the previous two points, x_{i-1} and x_{i-2} , is derived similarly. It is done by writing the three-term Taylor series expansion with a remainder, for the value of the function at point x_{i-1} and at point x_{i-2} , in terms of the value of the function and its derivatives at point x_i . The equations are then manipulated to obtain an equation without the terms that include the first derivative, which is then solved for $f''(x_i)$. The resulting formula is

$$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2} + O(h). \quad (19)$$

Three-point central difference formulas for the second derivative. Central difference formulas for approximating the second derivative can be constructed by incorporating an arbitrary number of points on either side of the evaluation point x_i . These formulas are derived by expressing the Taylor series expansion, including a remainder term, for points adjacent to x_i in terms of the function's value and its derivatives at x_i . Then, the equations are combined in such a way that the terms containing the first derivatives are eliminated. For instance, consider the four-term Taylor series expansion with a

remainder for the points x_{i+1} and x_{i-1}

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_1)}{4!}h^4, \quad \xi_1 \in]x_i, x_{i+1}[, \quad (20)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_2)}{4!}h^4, \quad \xi_2 \in]x_{i-1}, x_i[. \quad (21)$$

Adding (20) and (21) gives

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)h^2 + \frac{f^{(4)}(\xi_1)}{4!}h^4 + \frac{f^{(4)}(\xi_2)}{4!}h^4. \quad (22)$$

An estimate for the second derivative can be obtained by solving (22) for $f''(x_i)$ while neglecting the remainder terms. This introduces a truncation error of the order of h^2 .

$$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2} + O(h). \quad (23)$$

Equation (23) is the three-point central difference formula that provides an estimate of the second derivative at point x_i from the value of the function at that point, at the previous point, x_{i-1} , and at the next point x_{i+1} , with a truncation error of $O(h^2)$.

Formulas for higher-order derivatives can be derived by using the same procedure that are used here for the second derivative. For instance, the fourth-order accurate formula involving the five points x_{i-2} , x_{i-1} , x_i , x_{i+1} and x_{i+2} :

$$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2} + O(h^4). \quad (24)$$

A list of such formulas is given in below.

Example 1

1 Use a forward, backward and central difference and the values of h shown, to approximate the derivative of $\cos(x)$ at $x = \pi/3$

$$(a) \quad h = 0.1, \quad (b) \quad h = 0.01, \quad (c) \quad h = 0.001, \quad (d) \quad h = 0.0001.$$

2 Calculate the second derivative of $f(x) = 5^x/x$ at $x = 2$ numerically with the three-point central difference formula using the points

$$(a) \quad x = 1.8, \quad x = 2, \quad x = 2.2 \quad (b) \quad x = 1.9, \quad x = 2, \quad x = 2.1$$

Example 2

Consider the oscillatory function $v(x) = e^{-x/7} \sin(23x)$. Find the value of :

- a The first derivative at $x = 2$ using the four-point central difference formula with $x_{i-2} = 1.96$, $x_{i-1} = 1.98$, $x_{i+1} = 2.02$ and $x_{i+2} = 2.04$. Compare with the analytical differentiation by hand.
- b The second derivative at $x = 2$ using the five-point central difference formula with $x_{i-2} = 1.96$, $x_{i-1} = 1.98$, $x_i = 2$, $x_{i+1} = 2.02$ and $x_{i+2} = 2.04$. Compare with the analytical differentiation.

Example 3

Using a four-term Taylor series expansion, derive a four-point backward difference formula for evaluating the first derivative of a function given by a set of unequally spaced points.

(The formula should give the derivative at point x_i in terms of x_i , x_{i-1} , x_{i-2} , x_{i-3} , $f(x_i)$, $f(x_{i-1})$, $f(x_{i-2})$ and $f(x_{i-3})$).

Example 4

Derive a finite difference approximation formula for $f''(x_i)$ using three points x_{i-1} , x_i , x_{i+1} , where the spacing is such that $x_i - x_{i-1} = 2h$ and $x_{i+1} - x_i = h$.

Example 5

- a Let $f : [a, b] \rightarrow \mathbb{R}$ be a function of class at least C^5 on the interval $[a, b]$. Fix a “small” number $h > 0$ and an arbitrary point $x \in (a, b)$. Show that the ratio A approaches a derivative of f (which we will determine), then state the order of accuracy of this approximation in each case

$$A = \frac{-f(x + 2h) + 8f(x + h) - 8f(x - h) + f(x - 2h)}{12h}$$

$$A = \frac{f(x + 3h) - 3f(x + h) + 3f(x - h) - f(x - 3h)}{8h^3}$$

- b Suppose now that f be of class at least C^6 , repeat the same question with the following ratios

$$B = \frac{-f(x + 2h) - 4f(x + h) + 6f(x) - 4f(x - h) + f(x - 2h)}{h^4}$$

$$B = \frac{-2f(x + 2h) - 32f(x + h) - 60f(x) + 32f(x - h) - 2f(x - 2h)}{24h^2}$$

Finite difference formulas: First Derivative

Method	Formula	Error
2point Forward D	$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
3point Forward D	$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
2point Backward D	$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
3point Backward D	$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
2point Central D	$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h)$
4point Central D	$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

Finite difference formulas: Second Derivative

Method	Formula	Error
3point Forward D	$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
4point Forward D	$f''(x_i) = \frac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
3point Backward D	$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h}$	$O(h)$
4point Backward D	$f''(x_i) = \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
3point Central D	$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
5point Central D	$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

Sect.4 Differentiation Formulas using Lagrange Polynomials

The differentiation formulas can alternatively be derived through the application of Lagrange polynomials. Specifically, the first derivative, the two-point central, three-point forward, and three-point backward difference formulas are obtained by considering three points (x_i, y_i) , (x_{i+1}, y_{i+1}) and (x_{i+2}, y_{i+2}) . The interpolating polynomial that traverses these points, expressed in Lagrange form, is defined as follows:

$$f(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2} \quad (25)$$

Differentiating (25) gives:

$$f'(x) = \frac{2x - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{2x - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{2x - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2} \quad (26)$$

The first derivative at either one of the three points is calculated by substituting the corresponding value of x (x_i , x_{i+1} or x_{i+2}) (26). This gives the following three formulas for the first derivative at the three points

$$\begin{aligned} f'(x_i) &= \frac{2x_i - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2} \\ f'(x_{i+1}) &= \frac{x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{2x_{i+1} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{x_{i+1} - x_i}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2} \\ f'(x_{i+2}) &= \frac{x_{i+2} - x_{i+1}}{(x_i - x_{i+1})(x_i - x_{i+2})}y_i + \frac{x_{i+2} - x_i}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}y_{i+1} + \frac{2x_{i+2} - x_{i+1} - x_i}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}y_{i+2} \end{aligned}$$

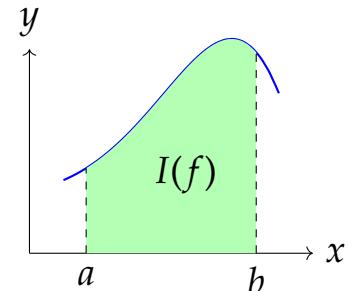
It is worthy to notice that if the points are equally spaced, the latter formulas reduce to the three-point forward difference formula (16), the two-point central difference formula (12) and the three-point backward difference formula (17), respectively. Furthermore, equation (26) has two other important features. It can be used when the points are not spaced equally, and it can be used for calculating the value of the first derivative at any point between x_i and x_{i+2} .

Example 6

Use Lagrange interpolation polynomials to find the finite difference formula for the second derivative at the point x_i using the unequally spaced points x_i , x_{i+1} and x_{i+2} . What is the second derivative at x_{i+1} and x_{i+2} ?

Sect.5 Numerical Integration

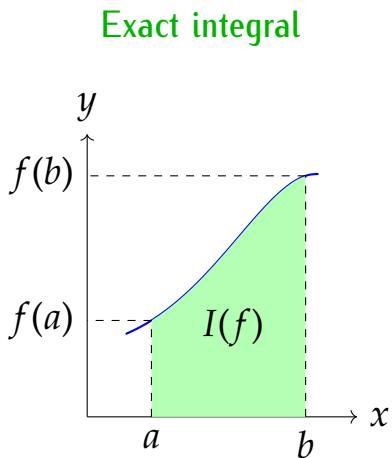
Numerical evaluation of a single integral deals with estimating the number $I(f)$ that is the integral of a function $f(x)$ over an interval from a and b . If the integrand $f(x)$ is an analytical function, the numerical integration is done by using a finite number of points at which the integrand is evaluated.



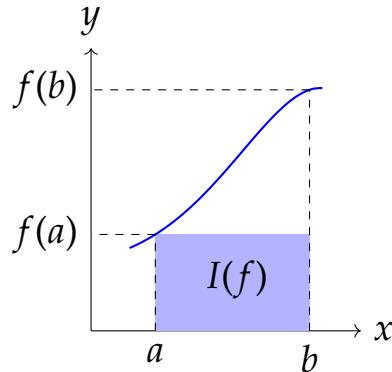
Higher accuracy can be achieved by using a composite method where the interval $[a, b]$ is divided into smaller subintervals. The integral over each subinterval is calculated, and the results are added together to give the value of the whole integral. If the integrand $f(x)$ is given as a set of discrete points (tabulated data), the numerical integration is done by using these points.

Sect.6 Rectangle and Midpoints Methods

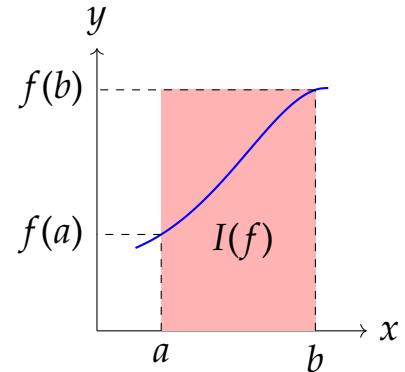
The simplest approximation for $\int_a^b f(x)dx$ is to take $f(x)$ over the interval $x \in [a, b]$ as a constant equal to the value of $f(x)$ at either one of the endpoints.



Approximation of integral assuming $f(x) = f(a)$



Approximation of integral assuming $f(x) = f(b)$



The integral can then be calculated in one of two ways:

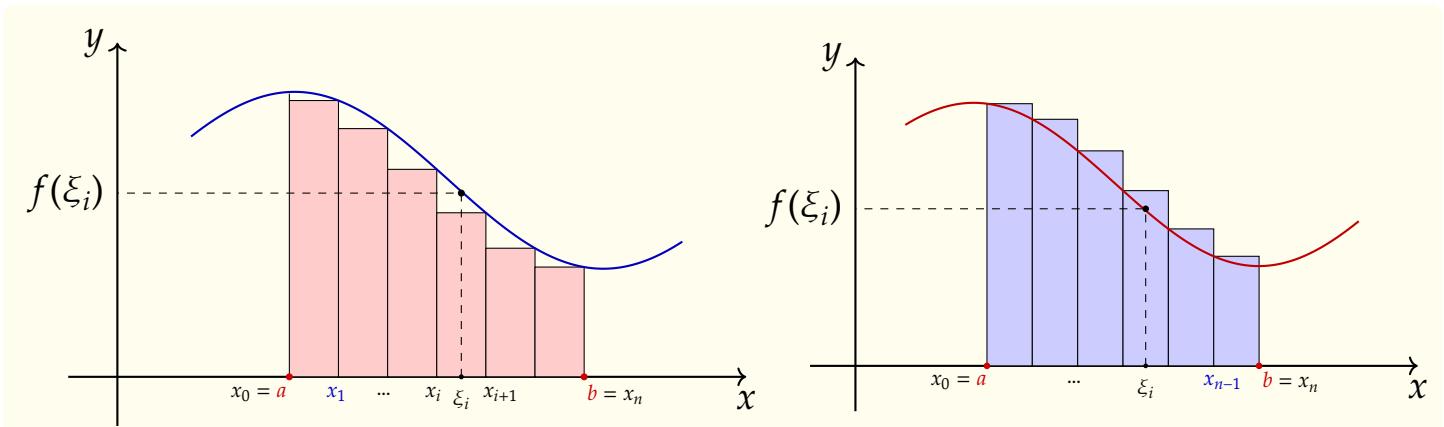
$$I(f) = \int_a^b f(x)dx = f(a)(b - a) \quad \text{or} \quad I(f) = \int_a^b f(x)dx = f(b)(b - a)$$

Obviously for the monotonically increasing function shown, the value of the integral is underestimated when $f(x)$ is assumed to be equal to $f(a)$, and overestimated when $f(x)$ is assumed to be equal to

$f(b)$. Therefore, the error can be large. Besides, when the integrand is an analytical function, the error can be significantly reduced by using the composite rectangle method.

Composite rectangle method

In the composite rectangle method the domain $[a, b]$ is divided into n subintervals by defining the x_0, x_1, \dots, x_n . The first point is $x_0 = a$ while the last point is $x_n = b$. The integral in each subinterval is calculated with the rectangle method, and the value of the whole integral is obtained by adding the values of the integrals in the subintervals. Certainly, this shows that the subintervals have the same width, but in general, subintervals can have arbitrary width.



When the integrand in each subinterval is assumed to have the value of the integrand at the beginning of the subinterval, then the integral over the whole domain can be written as the sum of the integrals in the subintervals as follows

$$\begin{aligned} I(f) &= \int_a^b f(x)dx \approx \overbrace{f(x_0)(x_1 - x_0)}^{I_1} + \overbrace{f(x_1)(x_2 - x_1)}^{I_2} + \cdots + \overbrace{f(x_{n-1})(x_n - x_{n-1})}^{I_n} \\ &= \sum_{i=0}^{n-1} f(x_i)(x_{i+1} - x_i) \end{aligned} \quad (27)$$

When the subintervals have the same width $x_{i+1} - x_i = h$, the latter equation can be simplified to

$$I(f) = \int_a^b f(x)dx \approx h \sum_{i=0}^{n-1} f(x_i) \quad (28)$$

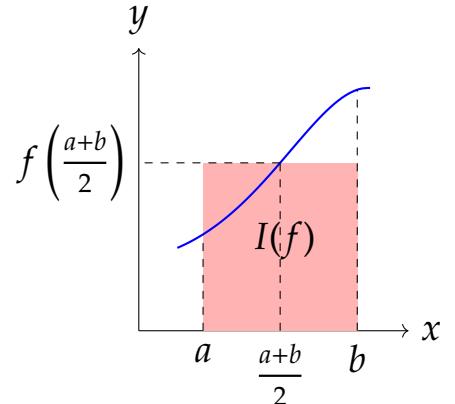
Equation (28) is the formula for the composite rectangle method for the case where the subintervals have identical width h .

Midpoint method

An improvement over the naive rectangle method is the midpoint method. Instead of approximating the integrand by the values of the function at $x = a$ or $x = b$, the value of the integrand at the middle of the interval, that is, $f((a + b)/2)$ is used. In this case, the approximation of integral is

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

The midpoint method



As depicted graphically, the integral is estimated by replacing the curve with a single rectangle of equal area. For functions that only increase or decrease, this works better than basic rectangle methods because overestimates and underestimates tend to cancel out. However, this balance isn't guaranteed for all functions. To improve accuracy, split the area into smaller sections and use midpoint rectangles for each.

Composite midpoint method

In the composite midpoint method, the domain $[a, b]$ is divided into n subintervals. The integral in each subinterval is calculated with the midpoint method and the value of the whole integral is obtained by adding the values of the integrals in the subintervals. As above, by using the value of the integrand at the middle of each subinterval, the integral over the whole domain can be written as the sum of the integrals in the subintervals as follows

$$I(f) = \int_a^b f(x)dx \approx \overbrace{f\left(\frac{x_0+x_1}{2}\right)(x_1-x_0)}^{I_1} + \overbrace{f\left(\frac{x_1+x_2}{2}\right)(x_2-x_1)}^{I_2} + \cdots + \overbrace{f\left(\frac{x_{n-1}+x_n}{2}\right)(x_n-x_{n-1})}^{I_n} = \sum_{i=0}^{n-1} f\left(\frac{x_i+x_{i+1}}{2}\right)(x_{i+1}-x_i) \quad (29)$$

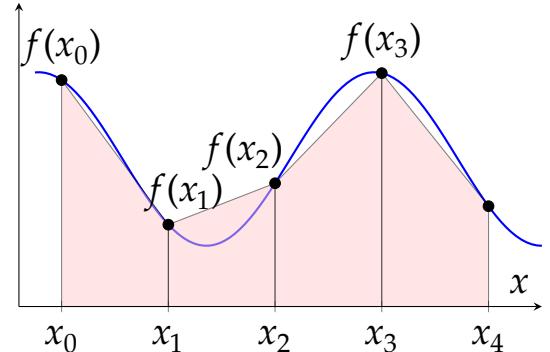
When the subintervals have the same width $x_{i+1} - x_i = h$, the equation (29) can be simplified to

$$I(f) = \int_a^b f(x)dx \approx h \sum_{i=0}^{n-1} f\left(\frac{x_i+x_{i+1}}{2}\right) \quad (30)$$

Equation (30) is the formula for the composite midpoint method for the case where the subintervals have identical width h .

Sect.7 Trapezoid Method

For greater accuracy than basic rectangle or midpoint methods, we can approximate the integrand with straight-line segments over each integration interval (by linear interpolation). Visually replacing rectangles with trapezoids, this method improves on rectangle/midpoint approaches by using linear approximations over each interval.



Newton's form of interpolating polynomials with two points $x_0 = a$ and $x_1 = b$, yields

$$f(x) \approx f(a) + (x - a)f[a, b] = f(a) + (x - a) \left(\frac{f(b) - f(a)}{b - a} \right) \quad (31)$$

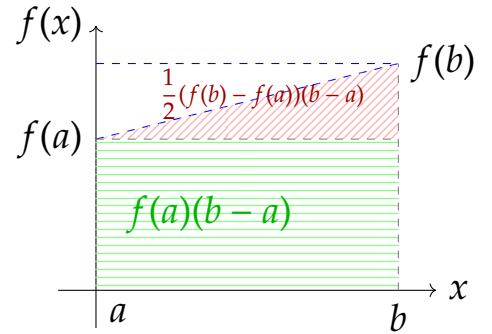
In this case, the integral $I(f)$ becomes

$$I(f) \approx \int_a^b \left(f(a) + (x - a) \left(\frac{f(b) - f(a)}{b - a} \right) \right) dx = \frac{1}{2}(b - a) (f(b) + f(a)). \quad (32)$$

The simplified trapezoidal rule decomposes into two areas:

- a $f(a)(b - a)$ [rectangle: height $f(a)$, width $b - a$],
- b $\frac{1}{2}(b - a)(f(b) - f(a))$ [triangle: base $b - a$, height $f(b) - f(a)$].

As the figure shows, their sum creates a trapezoid approximating $\int_a^b f(x)dx$ a more accurate alternative to single-rectangle methods.



Composite Trapezoidal Method

As with the rectangle and midpoint methods, the trapezoidal method can be easily extended to yield any desired level of accuracy by subdividing the interval $[a, b]$ into n subintervals by defining the x_0, x_1, \dots, x_n . The first point is $x_0 = a$ while the last point is $x_n = b$. The integral over the whole interval can be written as the sum of the integrals in the subintervals

$$I(f) = \int_a^b f(x)dx \approx \overbrace{\int_{x_0=a}^{x_1} f(x)dx}^{I_1} + \overbrace{\int_{x_1}^{x_2} f(x)dx}^{I_2} + \cdots + \overbrace{\int_{x_{n-1}}^{x_n} f(x)dx}^{I_n} = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx. \quad (33)$$

Applying the trapezoidal method to each subinterval $[x_i, x_{i+1}]$ yields

$$I_i(f) = \int_{x_i}^{x_{i+1}} f(x)dx = \frac{1}{2} (f(x_{i+1}) + f(x_i))(x_{i+1} - x_i).$$

Substituting the trapezoidal approximation in the right side of (33) gives

$$I(f) = \int_a^b f(x)dx \approx \frac{1}{2} \sum_{i=0}^{n-1} (f(x_{i+1}) + f(x_i))(x_{i+1} - x_i). \quad (34)$$

Notice that (34) is the general formula for the composite trapezoidal method where the subintervals $[x_i, x_{i+1}]$ need not be identical at all. However, if the subintervals are all the same width, that is, if

$$x_n - x_{n-1} = \cdots = x_1 - x_0 = h$$

then (34) can be simplified to

$$\begin{aligned} I(f) &= \int_a^b f(x)dx \approx \frac{h}{2} \sum_{i=0}^{n-1} (f(x_{i+1}) + f(x_i)) = \frac{h}{2} (f(a) + 2f(x_1) + \cdots + 2f(x_{i-1}) + f(b)) \\ &= \frac{h}{2} (f(a) + f(b)) + h \sum_{i=1}^{n-1} f(x_i). \end{aligned} \quad (35)$$

Example 7

Approximate $\int_0^1 e^{-x^2} dx$ with $n = 5$ (six points $x_0 = 0$ and $x_5 = 1$). Therefore,

$$h = 0.2, \quad x_i = \{0, 0.2, 0.4, 0.6, 0.8, 1\}, \quad f(x_i) = e^{-x_i^2}$$

$$\int_0^1 e^{-x^2} dx \approx \frac{0.2}{2} (f(0) + 2 \sum_{i=1}^4 f(x_i) + f(1)) = 0.7444$$

Sect.8 Simpson's Method

While the trapezoidal method uses linear approximations for numerical integration, higher accuracy can be achieved through nonlinear function approximations that remain simple to integrate. Simpson's rules provide this enhanced precision by employing polynomial approximations:

- a Simpson's 1/3 method uses quadratic polynomials.
- b Simpson's 3/8 method uses cubic polynomials.

Sect.8.1 Simpson's 1/3 Method

In this method, a quadratic polynomial is used to approximate the integrand using three points, i.e. the two endpoints $x_0 = a$ and $x_2 = b$, and the midpoint $x_1 = \frac{a+b}{2}$. Notice that, in this case, we have

$$b - \frac{a+b}{2} = \frac{a+b}{2} - a = \frac{b-a}{2} = h.$$

The Newton polynomial can be written in the form

$$P(x) = a + b(x - x_0) + c(x - x_0)(x - x_1)$$

Using next the fact that $P(x_i) = f(x_i)$ we deduce that

$$P_2(x) = f(a) + 2 \left[\frac{f(x_1) - f(a)}{b - a} \right] (x - a) + \left[\frac{f(a) - 2f(x_1) + f(b)}{(b - a)^2} \right] (x - a)(2x - a - b)$$

Therefore, by integrating $P_2(x)$ over $[a, b]$ gives

$$I(f) = \int_{x_0}^{x_2} f(x) dx \approx \int_{x_0}^{x_2} P_2(x) dx = \frac{h}{3} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right) \quad (36)$$

If we use the Lagrange polynomials, we shall write

$$P_2(x) = f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x)$$

with

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \implies \int_a^b L_0(x) dx = \frac{b - a}{6} = \frac{h}{3}$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \implies \int_a^b L_1(x) dx = \frac{4(b - a)}{6} = \frac{4h}{3}$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} \implies \int_a^b L_2(x) dx = \frac{b - a}{6} = \frac{h}{3}$$

we then get the integral over $[a = x_0, x_2 = b]$ we obtain again (36). The name 1/3 in the method comes from the fact that there is a factor of 1/3 multiplying the expression in the brackets in (36).

Composite Simpson's 1/3 Method

The composite Simpson's 1/3 method, offering improved accuracy over rectangular and trapezoidal approaches, works by segmenting $[a, b]$ into n subintervals. Our derivation focuses on the case

where these subintervals have equal width $h = (b - a)/n$. Since Simpson's 1/3 rule integrates over two subintervals simultaneously (first+second, third+fourth, etc.), the total number of subintervals n must be even. The overall integral is calculated as the combination of the integrals evaluated over each such pair.

$$I(f) = \int_a^b f(x)dx \approx \int_{x_0=a}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n=b} f(x)dx \quad (37)$$

By using (36), the integral over two adjacent intervals $[x_{i-2}, x_{i-1}]$ and $[x_{i-1}, x_i]$ can be written in terms of the Simpson's 1/3 method as

$$I_i(f) = \int_{x_{i-2}}^{x_i} f(x)dx \approx \frac{h}{3} [f(x_{i-2}) + 4f(x_{i-1}) + f(x_i)] \quad (38)$$

where $h = x_i - x_{i-1} = x_{i-1} - x_{i-2}$. Using (38) for each of the integrals in (37) we obtain

$$I(f) \approx \frac{h}{3} [f(a) + 4f(x_1) + f(x_2) + f(x_2) + 4f(x_3) + f(x_4) + \cdots + f(x_{n-2}) + 4f(x_{n-1}) + f(b)]$$

By collecting similar terms, the right side of the last equation can be simplified to give the general equation for the composite Simpson's 1/3 method for equally spaced subintervals with $h = (b - a)/n$

$$I(f) \approx \frac{h}{3} \left[f(a) + 4 \sum_{i=1,3,\dots}^{n-1} f(x_i) + 2 \sum_{i=2,4,\dots}^{n-2} f(x_j) + f(b) \right]. \quad (39)$$

Introducing the nodes $x_k = a + k(b - a)/2m$, for $0 \leq k \leq 2m$, $m \geq 1$, the latter formula maybe written in the following compact expression

$$I(f) \approx \frac{h}{3} \left[f(a) + 4 \sum_{s=0}^{m-1} f(x_{2s+1}) + 2 \sum_{r=1}^{n-1} f(x_{2r}) + f(b) \right]. \quad (40)$$

Equation (39) and equivalently (40) is the composite Simpson's 1/3 formula for numerical integration. It is important to point out that (39) can be used only if two conditions are satisfied:

- The subintervals must be equally spaced.
- The number of subintervals within $[a, b]$ must be an even number.

Example 8

Let us employ the midpoint, trapezoidal and Simpson's 1/3 composite formulae to compute

$$\text{a} \quad \int_0^{2\pi} x^2 e^{-x} \cos(7x) dx, \quad \text{b} \quad \int_0^{3.7} \frac{3+x^2}{1+7x^4} dx$$

Sect.8.2 Simpson's 3/8 Method

In this method a cubic polynomial is used to approximate the integrand using four points. For an integral over the domain $[a, b]$, the four points used are the two endpoints $x_0 = a$ and $x_3 = b$, and two points x_1 and x_2 that divide the interval into three equal sections with step size $h = (b - a)/3$. Therefore, $x_1 = a + h$ and $x_2 = a + 2h$. Apply the transformation:

$$t = \frac{x - a}{h} \quad \text{so that} \quad dx = hdt$$

When $x = a$, $t = 0$ and when $x = b$, $t = 3$. The integral becomes:

$$\int_a^b f(x)dx = h \int_0^3 f(a + th)dt$$

Construct the cubic polynomial $P_3(t)$ that interpolates f at $t = 0, 1, 2, 3$:

$$P_3(t) = \sum_{k=0}^3 f(x_k)L_k(t)$$

where $L_k(t)$ are the Lagrange basis polynomials:

$$L_0(t) = \frac{(t-1)(t-2)(t-3)}{(0-1)(0-2)(0-3)} = -\frac{1}{6}(t-1)(t-2)(t-3) \implies \int_0^3 L_0(t)dt = \frac{3}{8}$$

$$L_1(t) = \frac{(t-0)(t-2)(t-3)}{(1-0)(1-2)(1-3)} = \frac{1}{2}t(t-2)(t-3) \implies \int_0^3 L_1(t)dt = \frac{9}{8}$$

$$L_2(t) = \frac{(t-0)(t-1)(t-3)}{(2-0)(2-1)(2-3)} = -\frac{1}{2}t(t-1)(t-3) \implies \int_0^3 L_2(t)dt = \frac{9}{8}$$

$$L_3(t) = \frac{(t-0)(t-1)(t-2)}{(3-0)(3-1)(3-2)} = \frac{1}{6}t(t-1)(t-2) \implies \int_0^3 L_3(t)dt = \frac{3}{8}$$

The integral approximation becomes

$$\begin{aligned} \int_0^3 P_3(t)dt &= \sum_{k=0}^3 f(x_k) \int_0^3 L_k(t)dt = f(x_0) \cdot \frac{3}{8} + f(x_1) \cdot \frac{9}{8} + f(x_2) \cdot \frac{9}{8} + f(x_3) \cdot \frac{3}{8} \\ &= \frac{3}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] \end{aligned}$$

Multiply by h to transform back to x -coordinates:

$$\int_a^b f(x)dx \approx \frac{3h}{8} [f(a) + 3f(x_1) + 3f(x_2) + f(b)] \quad (41)$$

which is the Simpson's 3/8 rule.

Composite Simpson's 3/8 Method

In the composite Simpson's 3/8 method, the whole interval $[a, b]$ is divided into n subintervals. In general, the subintervals can have arbitrary width. The derivation here, however, is limited to the case where the subintervals have an equal width h where $(b - a)/n$. Since four points are needed for constructing a cubic polynomial, the Simpson's 3/8 method is applied to three adjacent subintervals at a time (the first three, the fourth, fifth, and sixth intervals together, and so on). Consequently, the whole interval has to be divided into a number of subintervals that is divisible by 3. The integration in each group of three adjacent subintervals is evaluated by using (41). Assume $n = 3m$, $m \geq 1$, then $x_k = a + k(b - a)/3m$, for $0 \leq k \leq 3m$. The integral over the whole domain is obtained by adding the integrals in the subinterval groups

$$I(f) = \int_a^b f(x)dx \approx \int_{x_0=a}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x_{3(m-1)}}^{x_{3m}=b} f(x)dx \quad (42)$$

By (41), for the segment k ($k = 0, 1, \dots, m - 1$), the integral over each interval $[x_{3i}, x_{3(i+1)}]$ can be written in terms of the Simpson's 1/3 method as

$$I_i(f) = \int_{x_{3i}}^{x_{3i+3}} f(x)dx \approx \frac{3h}{8} [f(x_{3i}) + 3f(x_{3i+1}) + 3f(x_{3i+2}) + f(x_{3i+3})]. \quad (43)$$

Using (43) for each of the integrals in (42), sum over all segments, we obtain the compact expression

$$\int_a^b f(x)dx \approx \frac{3h}{8} \left[f(a) + 3 \sum_{s=0}^{m-1} (f(x_{3s+1}) + f(x_{3s+2})) + 2 \sum_{r=1}^{n-1} f(x_{3r}) + f(b) \right]. \quad (44)$$

Example 9

A rocket is launched vertically from the ground and we measure its acceleration γ during the first 80 seconds. Determine the velocity V of the rocket at time $t = 80s$, using the trapezoidal rule and then Simpson's 1/3 and 3/8 rule.

t (in s)	0	10	20	30	40	50	60	70	80
γ (in m/s^2)	30	31.66	33.44	35.47	37.75	40.33	43.29	46.7	50.67

It is known that acceleration is defined as the time derivative of velocity V . Therefore,

$$V(t) = \int_0^{80} \gamma(s)ds \approx \dots$$

Sect.9 Convergence theorem and errors

Theorem 1

Let f be continuous in $[a, b]$. Then

$$\left| \int_a^b f(x)dx - h \sum_{k=0}^{n-1} f(a + kh) \right| \leq (b - a)w\left(\frac{b - a}{n}\right)$$

where $w(\delta)$ is the modulus of continuity of f defined by

$$w(\delta) = \max_{|x_1 - x_2| \leq \delta} |f(x_1) - f(x_2)|, \quad a \leq x_1, x_2 \leq b$$

Proof. We have

$$\left| \int_a^b f(x)dx - h \sum_{k=0}^{n-1} f(a + kh) \right| = \sum_{k=0}^{n-1} \int_{a+kh}^{a+(k+1)h} (f(x) - f(a + kh)) dx$$

Now, for $a + kh \leq x \leq a + (k + 1)h$, we have

$$|f(x) - f(a + kh)| \leq w(h) \implies \left| \int_{a+kh}^{a+(k+1)h} (f(x) - f(a + kh)) dx \right| \leq hw(h)$$

Therefore, by adding n of these inequalities, we obtain

$$\left| \int_a^b f(x)dx - h \sum_{k=0}^{n-1} f(a + kh) \right| \leq nhw(h) = hw\left(\frac{b - a}{n}\right) \quad \square$$

The trapezoidal and midpoint rules are exact for linear functions and converge at least as fast as n^{-2} , if we assume that the integrand has a continuous second derivative.

Theorem 2

Let $f(x) \in C^2([a, b])$. Then

$$\int_a^b f(x)dx - \frac{h}{2} \left(f(a) + 2 \sum_{i=1}^{n-1} f(a + ih) + f(b) \right) = -\frac{(b - a)^3}{12n^2} f'''(\xi), \quad a < \xi < b.$$

$$\int_a^b f(x)dx - h \sum_{i=1}^{n-1} f\left(a + \frac{2k+1}{2}h\right) = \frac{(b - a)^3}{12n^2} f'''(\xi), \quad a < \xi < b.$$

Sect.10 Gaussian Quadrature

Gaussian quadrature is a numerical integration method that uses a higher order of interpolation than do either the trapezoidal or Simpson rules. A detailed derivation of the method is rather involved as it relies on Hermite interpolation, orthogonal polynomial theory, and some aspects of the theory rely on issues relating to linear system solution. Most quadrature formulas take the form

$$I(f) \approx I_n(f) = \sum_{i=0}^n w_i f(x_i)$$

where x_i are the quadrature points, or abscissas, and the w_i are called the quadrature weights. Generally, there are two approaches which can be taken to develop numerical quadrature formulas. In the first approach, the x_i are fixed, typically as equally spaced points from within the interval $[a, b]$, and the w_i are computed by fitting a function to the $f(x_i)$ data and integrating the resulting function exactly. When the chosen interpolating function is a polynomial, a Newton-Cotes Quadrature rule is obtained. In the second approach, given the number of data points n , the weights and abscissas of the quadrature rule are selected to achieve maximum possible accuracy. Formulas developed in this manner are known as Gaussian Quadrature rule.

Degree of Precision (Accuracy)

Like the error term associated with a difference approximation, the error term associated with quadrature rule provides two pieces of information. First, the error term indicates precisely how the error depends on the length of the integration interval. Second, the error term allows us to determine the degree of precision, which characterizes the class of polynomials for which the quadrature formula produces exact results.

Definition 1

The degree of precision (or accuracy) of a quadrature rule $I_n(f)$ is the positive number m such that

- ✓ $I(p) = I_n(p)$ for every polynomial p of degree $\leq m$.
- ✓ $I(p) \neq I_n(p)$ for some polynomial p of degree $m + 1$.

Example 10

The following table demonstrates explicitly that the Trapezoid rule integrates 1 and x exactly, but fails to integrate x^2 exactly, hence the degree of precision is 1

$f(x)$	$\int_a^b f(x)dx$	$h[f(a) + f(a + h)]/2$
1	$b - a$	$b - a$
x	$(b^2 - a^2)/2$	$(b^2 - a^2)/2$
x^2	$(b^3 - a^3)/3$	$(b^3 - a^3 + ba^2 - ab^2)/3$

Example 11

The degree of precision of Simpson's 1/3 rule is three:

$f(x)$	$\int_a^b f(x)dx$	$\frac{h}{3} [f(a) + f(a + h) + f(a + 2h)]$
1	$b - a$	$b - a$
x	$(b^2 - a^2)/2$	$(b^2 - a^2)/2$
x^2	$(b^3 - a^3)/3$	$(b^3 - a^3)/3$
x^3	$(b^4 - a^4)/4$	$(b^4 - a^4)/4$
x^4	$(b^5 - a^5)/5$	$(5b^5 - b^4a + 2b^3a^2 - 2b^2a^3 + ba^4 - 5a^5)/24$

Exercise 1

Determine values A_0 , A_1 and A_2 so that the following quadrature formulas has degree of precision at least 2

- a $\int_{-1}^1 f(x)dx = A_0 f\left(-\frac{1}{2}\right) + A_1 f(0) + A_2 f\left(\frac{1}{2}\right)$
- b $\int_{-1}^1 f(x)dx = A_0 f\left(-\frac{1}{3}\right) + A_1 f(0) + A_2 f\left(\frac{1}{3}\right)$
- c $\int_{-1}^1 f(x)dx = A_0 f(-1) + A_1 f(A_2)$

Solution

To determine the values of A_0 , A_1 and A_2 such that the quadrature formula has a degree of precision at least 2, the formula must be exact for all polynomials of degree at most 2. This

requires the formula to hold for the monomials $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$.

$$f(x) = 1 : \quad \int_{-1}^1 dx = 2 = A_0 + A_1 + A_2$$

$$f(x) = x : \quad \int_{-1}^1 x dx = 0 = A_0 \left(-\frac{1}{2} \right) + A_1 \cdot 0 + A_2 \left(\frac{1}{2} \right) \implies A_0 = A_2$$

$$f(x) = x^2 : \quad \int_{-1}^1 x^2 dx = \frac{2}{3} = A_0 \left(-\frac{1}{2} \right)^2 + A_1 \cdot 0 + A_2 \left(\frac{1}{2} \right)^2 \implies A_0 + A_2 = \frac{8}{3}$$

Method of Undetermined Coefficients

The method of undetermined coefficients is essentially the brute force method for developing Gaussian quadrature rules. It involves a straightforward application of the definition of the degree of precision and proceeds as follows. Given a positive integer n , we wish to determine $2n$ numbers, the abscissas x_1, x_2, \dots, x_n and the weights w_1, w_2, \dots, w_n , so that the summation

$$w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n)$$

provides the exact values of $\int_a^b f(x) dx$ for $f(x) = 1, x, x^2, \dots, x^n$. In other words, the quadrature rule will have degree of precision equal to $2n - 1$. Applying each of these conditions produces a system of $2n$ equations, which will be nonlinear for all $n \geq 1$.

To demonstrate the method of undetermined coefficients process, let's develop a Gaussian quadrature rule with $n = 1$. We want the approximation formula

$$\int_a^b f(x) dx = w_1 f(x_1).$$

to have a degree of precision 1, that is, this formula should obtain exact results for all constant and for all linear functions. Applying these two conditions produces the following system of equations:

$$f(x) = 1 : \quad w_1 = \int_a^b dx = b - a$$

$$f(x) = x : \quad w_1 x_1 = \int_a^b x dx = \frac{1}{2} (b^2 - a^2)$$

The solution of this system is $w_1 = b - a$ and $x_1 = (a + b)/2$. The resulting Gaussian quadrature

rule is

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

which we should recognize as the midpoint rule.

In determining Gaussian quadrature rule with $n > 1$, it is to our advantage to replace the general integration interval $[a, b]$ with a standardized interval, the most common choice for which is $[-1, 1]$. With such an interval we can exploit the symmetries in the problem to simplify the solution of the nonlinear system of equations for the abscissas and weights. The conversion from the integral $\int_a^b f(x)dx$ to an integral of the form $\int_{-1}^1 \tilde{f}(x)dx$ is most easily accomplished by the change of variable

$$x = \frac{b-a}{2}t + \frac{a+b}{2}$$

The resulting relationship between the two integrals is then

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

Let's now construct the two-point Gaussian quadrature rule

$$\int_{-1}^1 f(x)dx \approx w_1 f(x_1) + w_2 f(x_2)$$

Since this formula is to have degree of precision equal to $2(2)-1=3$, the weights and abscissas must satisfy

$$f(x) = 1 : \quad w_1 + w_2 = \int_{-1}^1 dx = 2$$

$$f(x) = x : \quad w_1 x_1 + w_2 x_2 = \int_{-1}^1 x dx = 0$$

$$f(x) = x^2 : \quad w_1 x_1^2 + w_2 x_2^2 = \int_{-1}^1 x^2 dx = 2/3$$

$$f(x) = x^3 : \quad w_1 x_1^3 + w_2 x_2^3 = \int_{-1}^1 x^3 dx = 0$$

The symmetry of the integration interval about zero suggests $x_1 = -x_2$ and $w_1 = w_2$. Substituting these relations into the system, the equations $f(x) = x$ and $f(x) = x^3$ are satisfied exactly, and remaining equations take the form $2w_1 = 2$ and $2w_1 x_1^2 = 2/3$. The solution of the system is then $w_1 = w_2 = 1$ and $x_1 = -\sqrt{1/3}$ and $x_2 = \sqrt{1/3}$ giving the quadrature formula

$$\int_{-1}^1 f(x)dx \approx f\left(-\sqrt{\frac{1}{3}}\right) + f\left(\sqrt{\frac{1}{3}}\right)$$