8. Numerical Differentiation and Numerical Integration.

NUMERICAL ANALYSIS. Prof. Y. Nishidate (323-B, nisidate@u-aizu.ac.jp)
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NUMERICAL DIFFERENTIATION

Forward Difference Quotation

The most obvious way to approximate numerically the value of the derivative $f'(x)$ of a function $f(x)$ is to use the definition of derivative:

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

This approximation is called *forward difference quotient.* The first question that arises is how does the accuracy depend on h? If f is twice continuously differentiable, then from Taylor's theorem the *truncation error* is equal to:

$$\begin{aligned} E(h) &= (f(x) + hf'(x) + h^2 f''(\xi)/2 - f(x))/h - f'(x) \\ &= hf''(\xi)/2 = O(h) \end{aligned}$$

where $x \le \xi \le x+h$.

Central Difference Formula

If the function $f(x)$ can be evaluated at values to the left and to the right of x, then the best two-point formula involves symmetrical points:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

To get the trancation error we write down the Taylor expansions for $f(x+h)$ and $f(x-h)$

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \tfrac{h^2}{2!} f''(x) + \tfrac{h^3}{3!} f^{(3)}(\xi) \\ f(x-h) &= f(x) - hf'(x) + \tfrac{h^2}{2!} f''(x) - \tfrac{h^3}{3!} f^{(3)}(\xi) \end{aligned}$$

After subtraction of these two equations it is easy to obtain the trancation error:

$$E(h) = -\frac{h^2}{3!} f^{(3)}(\xi) = O(h^2)$$

Second Derivative

We can approximate values of the second derivative $f''(x)$ if we add the Taylor expansions for $f(x+h)$ and $f(x-h)$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

NUMERICAL INTEGRATION

Numerical integration methods are derived by integrating interpolation polynomials. Methods that are based on integrating the Newton interpolation formulas are called the Newton-Cotes integration formulas.

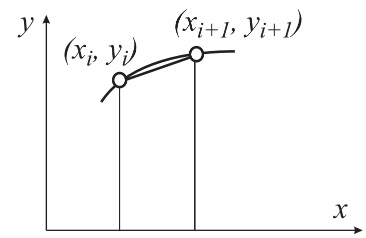
Trapezoidal rule

The trapezoidal rule is a numerical integration method derived by integrating the linear interpolation formula. It is written as

$$I = \int_{x_i}^{x_{i+1}} f(x)dx = \frac{f(x_i) + f(x_{i+1})}{2}\Delta x = \frac{h}{2}(f_i + f_{i+1})$$

where $\Delta x = h = x_{i+1} - x_i$. For the integration interval $[a, b]$ subdivided into n subintervals of size h the *composite trapezoidal rule* is as follows:

$$\begin{aligned} I &= \int_a^b f(x)dx = \sum_{i=0}^{n-1} \tfrac{h}{2}(f_i + f_{i+1}) \\ &= \tfrac{h}{2}(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{n-1} + f_n) \end{aligned}$$



It is possible to show that the local error (error for a single step of size h) is equal to:

$$e(h) = -\frac{1}{12}h^3 f''(\xi), \qquad x_1 < \xi < x_2$$

A global error of the composite trapezoidal rule is the summation of the errors for all the intervals:

$$E(h) = -\frac{1}{12}h^3 \sum_{i=1}^{n} f''(\xi_i) = O(h^2)$$

Romberg integration

We can improve the accuracy of the trapezoidal rule by a technique, which is known as *Romberg integration.* Suppose the result of the trapezoidal rule with point interval $h = (b-a)/n$ is I_h, and the result with $2h$ is I_{2h}. Since the error of the trapezoidal rule is proportional to h^2, the errors with intervals h and $2h$ may be written as

$$E(h) = ch^2 \qquad E(2h) = c(2h)^2$$

where c is a constant. On the other hand, the exact integral may be expressed as

$$I = I_h + E(h) = I_{2h} + E(2h)$$

or

$$E(h) - E(2h) = I_{2h} - I_h$$

Solving for c

$$c = \frac{1}{3h^2}(I_h - I_{2h})$$

and substituting we arrive at the following Romberg integration rule:

$$I = I_h + \frac{1}{3}(I_h - I_{2h})$$

which provides improved estimate of the integral based on integral values with intervals h and $2h$.

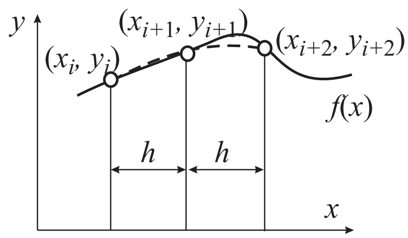
Simpson's 1/3 rule

Simpson's 1/3 rule is based on the quadratic interpolating polynomial. The general form of the equation of the second-degree parabola connecting three points is

$$y = ax^2 + bx + c$$

The integration of this equation from $-h$ to h gives the area contained in the two strips of integration:

$$I_{2\ strips} = \int_{-h}^{h} (ax^2 + bx + c)dx = \frac{2}{3}ah^3 + 2ch$$



The constants a and c can be determined from the fact that parabola should pass through points $(-h, y_i)$, $(0, y_{i+1})$ and (h, y_{i+2}):

$$\begin{aligned} y_i &= a(-h)^2 + b(-h) + c \\ y_{i+1} &= c \\ y_{i+2} &= ah^2 + bh + c \end{aligned}$$

Solving these equations and substituting constants we get

$$I_{2\ strips} = \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$$

If the area under a curve is divided into n uniform strips (n is even) the Simpson's one-third composite rule is as follows:

$$I = \tfrac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + ... + 2f_{n-2} + 4f_{n-1} + f_n) \\ +O(h^4)$$

Simpson's 3/8 rule

The composite rule based on fitting four points with a cubic leads to Simpson's 3/8 rule. We start with integral for three strips:

$$I_{3\ strips} = \frac{3h}{8}(f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3})$$

Applying this relation to interval consisting of sets of three strips we obtain the composite rule:

$$I = \tfrac{3h}{8}(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 \\ +... + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n) + O(h^4)$$

Gauss Quadrature

Our previous formulas for numerical integration were based on equally spaced x-coordinates of subintervals. A formula with three parameters (three points) corresponds to a polynomial of the second degree. Gauss observed that if we remove the requirements that the function be evaluated at predetermined x-values, then a three-term formula will contain six parameters (the three x-values and the three weight) and should correspond to an interpolating polynomial of degree 5. Formulas based on this principle are called *Gauss quadrature formulas*. They can be applied when $f(x)$ can be evaluated at any desired value of x. Let us consider the integral

$$I = \int_{-1}^{1} f(t)dt$$

and approximate this integration formula using two points as

$$I = w_1 f(t_1) + w_2 f(t_2)$$

where w_k are weights and t_k are coordinates to evaluate function value.
The integration formula derived above is the simplest member of the Gauss quadrature rules. Similarly, three, four, and five points formulae are written as follows

$$\begin{aligned} I &= w_1 f(t_1) + w_2 f(t_2) + w_3 f(t_3) \\ I &= w_1 f(t_1) + w_2 f(t_2) + w_3 f(t_3) + w_4 f(t_4) \\ I &= w_1 f(t_1) + w_2 f(t_2) + w_3 f(t_3) + w_4 f(t_4) + w_5 f(t_5) \end{aligned}$$

where abscissas and weights for Gauss integration rules with number of points n from two to five are given in table below.

n	t_i	w_i
2	$(-/+)0.577350269189626$	1
3	$(-/+)0.774596669241483$	0.555555555555556
	0	0.888888888888889
4	$(-/+)0.861136311594053$	0.347854845137454
	$(-/+)0.339981043584856$	0.652145154862546
5	$(-/+)0.906179845938664$	0.236926885056189
	$(-/+)0.538469310105683$	0.478628670499366
	0	0.568888888888889

In general, the Gauss quadrature rule is expressed as follows

$$I = \sum_{k=1}^{n} w_k f(t_k)$$

where n is the number of integration points, t_k are abscissas and w_i are the weights of integration.

Transformation of integration limits $[-1, 1] \to [a, b]$ The Gauss integration formula with integration limits [-1, 1] may be applied to any arbitrary interval $[a, b]$ using the transformation

$$x_k = \frac{1}{2}(b + a) + \frac{1}{2}(b - a)t_k$$

The Gauss quadrature rule becomes

$$\int_a^b f(x)dx = \frac{1}{2}(b - a)\sum_{k=1}^{n} w_k f(x_k)$$