Numerical differentiation

The formulation of the problem

The formulation of the problem

Let us suppose that the values of the differentiable function f are known at the points $x_0, x_{\pm 1} = x \pm h, x_{\pm 2} = x \pm 2h, \ldots$ $(h > 0)$. Let us denote these values by $f_0, f_{\pm 1}, f_{\pm 2}$, etc., respectively. We approximate the derivatives of the function at the point x. These derivatives will be denoted by f_0', f_0'', etc.

Def. 120. Let us denote an arbitrary derivative of the sufficiently smooth function f at the point x by Df. An approximation of this value is denoted by $\Delta f(h)$ (the approximation depends on the distance of the nodes). We say that the approximation $\Delta f(h)$ at the point x is of order p (at least) if there is a real numbet $K > 0$ such that

$$|Df - \Delta f(h)| \leq Kh^p.$$

(That is $|Df - \Delta f(h)| = O(h^p)$.)

Forward difference

Forward difference

Based on the definition of the differential quotient

$$f' \approx \frac{f_1 - f_0}{h} =: \Delta f_+.$$

Moreover, if $f \in C^2$ then we have

$$\Delta f_+ = \frac{f_1 - f_0}{h} = \frac{(f_0 + f_0' h + f''(\xi)h^2/2) - f_0}{h} = f_0' + f''(\xi)h/2.$$

This shows that the order of the forward difference approximation is 1, that is halving the step-size h the error will be halved.

Backward difference

Backward difference

Based on the definition of the differential quotient

$$f' \approx \frac{f_0 - f_{-1}}{h} =: \Delta f_- .$$

Moreover, if $f \in C^2$ then we have

$$\Delta f_- = \frac{f_0 - f_{-1}}{h} = \frac{f_0 - (f_0 - f_0' h + f''(\xi) h^2/2)}{h} = f_0' - f''(\xi) h/2.$$

This shows that this approximation is of first order.

Centered difference

Centered difference

Let us investigate the arithmetic mean of the two previous approximations.

$$\Delta f_c := \frac{\Delta f_+ + \Delta f_-}{2} = \frac{f_1 - f_{-1}}{2h}.$$

Let us apply Taylor expansion around the point x. Let $f \in C^3$.

$$\Delta f_c = \frac{f_1 - f_{-1}}{2h}$$
$$= \frac{f_0 + f_0' h + f_0'' h^2/2 + f'''(\xi_1) h^3/6}{2h}$$
$$- \frac{f_0 - f_0' h + f_0'' h^2/2 - f'''(\xi_2) h^3/6}{2h} = f_0' + f'''(\xi)\frac{h^2}{6}.$$

Thus, this approximation has order 2.

Approximation of the second derivative

Approximation of the second derivative

The second derivative is the derivative of the first derivative.

$$\Delta^2 f_c = \frac{\Delta f_+ - \Delta f_-}{h} = \frac{f_1 - 2f_0 + f_{-1}}{h^2}.$$

Let us apply Taylor expansion again around the point x. Let $f \in C^4$.

$$\Delta^2 f_c =$$

$$= \frac{f_0 + f_0' h + f_0'' h^2/2 + f_0''' h^3/6 + f''''(\xi_1) h^4/24}{h^2} - \frac{2f_0}{h^2}$$

$$+ \frac{f_0 - f_0' h + f_0'' h^2/2 - f_0''' h^3/6 + f''''(\xi_2) h^4/24}{h^2} = f_0'' + f''''(\xi)\frac{h^2}{12}.$$

Thus, the approximation has order 2.

Other approximations

Other approximations

Rmk. A fourth order centered approximation of the first derivative

$$\frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}.$$

Rmk. A second order forward and backward approximation of the first derivative

$$\frac{-3f_0 + 4f_1 - f_2}{2h}, \quad \frac{f_{-2} - 4f_{-1} + 3f_0}{2h}.$$

Rmk. The above formulas can be generalized easily to cases when the step-size is not equidistant.

Other approximations

Rmk.

- The derivative at x_0 of the polynomial fitted to the points $(x_0, f_0), (x_1, f_1)$ (at most first degree) is the same as the forward difference. The derivative at x_0 of the polynomial fitted to the points $(x_{-1}, f_{-1}), (x_0, f_0)$ (at most first degree) is the same as the backward difference.
- The derivative at x_0 of the polynomial fitted to the points $(x_{-1}, f_{-1}), (x_0, f_0), (x_1, f_1)$ (at most second degree) is the same as the centered difference, moreover, its second derivate gives the centered difference approximation of the second derivative.
- The derivative at x_0 of the third degree spline function fitted to the points $(x - h, f_{-1}), (x, f_0), (x + h, f_1)$ is the same as the the centered difference approximation of the first derivative.

Richardson extrapolation

Richardson extrapolation

 Lewis Fry Richardson (1881-1953, British, physicist, metheorologist, psichologist)

Let the two values of the forward difference approximations of a function f at the point x_0 be: $\Delta f_+(h)$ and $\Delta f_+(h/2)$.

$$\Delta f_+(h) = f_0' + f''(\xi_h)\frac{h}{2},$$

$$\Delta f_+(h/2) = f_0' + f''(\xi_{h/2})\frac{h}{4}.$$

If h is small then $\xi_{h/2} \approx \xi_h$. Thus the approximation $2\Delta f_+(h/2) - \Delta f_+(h)$ may give a higher order approximation to the derivative. Indeed, the order of this approximation is 2.

Numerical integration

Motivation

Necessity of numerical integration

Newton–Leibniz formula:

$$\int_a^b f(x)\,\mathrm{d}x = F(b) - F(a).$$

We cannot use this formula if

- we cannot give the antiderivative of the function in closed form (e.g. $\sin x/x$, $\sin x^2$, e^{-x^2}).
- the computation of the antiderivative is complicated and time consuming.
- we know the values of the function at certain points only (e.g. measurements).

Requirements

Let us suppose that the function f is integrable on the interval $[a, b]$, and that we know the values of the function at the nodes

$$a \leq x_0 < x_1 < \ldots < x_n \leq b.$$

Let these function values denoted by $f_0, \ldots, f_n$, respectively. Then we should give an estimation to the integral by the help of the nodes and the function values.

Expectations:

- The approximation must be calculated easily,
- When we refine the nodes then the approximations must tend to the exact integral value of the functions,
- For sufficiently smooth functions the convergence must be fast.

Quadrature formulas

Quadrature formula

Let us denote the exact definite integral of the integrable function f by $I(f)$ and let one of its approximations at the given nodes be

$$I_n(f) = \sum_{k=0}^{n} a_k f_k.$$

Both the coefficients a_k (the so-called weights) and the function values f_k may depend on the number and the location of the nodes. The above formula is called quadrature formula.

Quadrature formula

Def. 121. We say that a quadrature formula is closed if it uses the function values both at a and b. If it does not use these values then the quadrature formula is open.

Let h be the larges step size between two adjacent nodes.

Def. 122. We say that the convergence order of the quadrature formula $I_n(f)$ is $r \geq 1$ (at least), if $|I(f) - I_n(f)| = O(h^r)$.

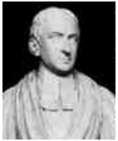
Def. 123. We say that the exactness order of the quadrature formula $I_n(f)$ is $r \geq 1$, if $I(p) = I_n(p)$ for all polynomials from P_{r-1} but there exists a polynomial p with degree r $(p \in P_r)$ such that $I(p) \neq I_n(p)$.

Newton–Cotes formulas

Newton–Cotes formulas

Def. 124. We call a quadrature formula interpolation quadrature formula, if it approximates the integral with the integral of the interpolation polynomial fitted to the given function values.

Def. 125. If in an interpolation quadrature formula the nodes are equidistant (h), then the formula is called to be a Newton–Cotes-formula.


Roger Cotes (1682-1716, angol)

Newton–Cotes formulas

The function f can be written in the form

$$f(x) = L_n(x) + r_n(x),$$

where L_n is the interpolation polynomial fitted to the function f on the given nodes, and r_n is the error term. Then the exact integral can be approximated as follows

$$I(f) = \int_a^b f(x)\,\mathrm{d}x = \int_a^b L_n(x)\,\mathrm{d}x + \int_a^b r_n(x)\,\mathrm{d}x$$

$$= \int_a^b \left(\sum_{k=0}^{n} f_k l_k(x) \right) \mathrm{d}x + \int_a^b r_n(x)\,\mathrm{d}x$$

$$= \underbrace{\sum_{k=0}^{n} f_k \left(\overbrace{\int_a^b l_k(x)\,\mathrm{d}x}^{a_k} \right)}_{I_n(f)} + \int_a^b r_n(x)\,\mathrm{d}x.$$

Newton–Cotes formulas

Here the weights depend on the interval of the integration. We can make them interval independent by changing the variable in the integral: let $x = a + (b-a)t$ ($t \in [0,1]$), thus $\mathrm{d}x/\mathrm{d}t = (b-a)$. In this way we have

$$a_k = \int_a^b l_k(x)\,\mathrm{d}x = \int_0^1 l_k(a+(b-a)t)(b-a)\,\mathrm{d}t$$
$$= (b-a)\int_0^1 l_k(a+(b-a)t)\,\mathrm{d}t,$$

where the last factor depends solely on the number of the interpolation nodes and their relative location. These values can be calculated and tabulated in advance: these are the so-called Newton–Cotes coefficients.

Closed Newton–Cotes formulas

With the setting

$$a = x_0 < x_1 < \ldots < x_n = b, \quad x_{k+1} - x_k = h = (b-a)/n$$

we obtain the weights

$$a_k = (b-a) N_{\mathsf{c}}^{n,k},$$

where the coefficients $N_{\mathsf{c}}^{n,k}$ are called closed Newton–Cotes coefficients.

$N_{\mathsf{c}}^{n,k}$	$k=0$	$k=1$	$k=2$	$k=3$	
$n=1$	$1/2$	$1/2$			$\leftarrow$ trapezoidal rule
$n=2$	$1/6$	$4/6$	$1/6$		$\leftarrow$ Simpson's rule
$n=3$	$1/8$	$3/8$	$3/8$	$1/8$	

Example. Applying the Simpson rule to

$$\int_1^3 x^2 - 2x + 2 \, \mathrm{d}x = 2(1 \cdot 1/6 + 2 \cdot 4/6 + 5 \cdot 1/6) = 14/3$$

we obtain the exact integral value.

Open Newton–Cotes formulas

With the setting

$$a = x_{-1} < x_0 < \ldots < x_n < x_{n+1} = b, \quad x_{k+1} - x_k = h = (b-a)/(n+2)$$

we obtain the weights

$$a_k = (b-a)N_\circ^{n,k},$$

where the coefficients $N_\circ^{n,k}$ are called open Newton–Cotes coefficients.

$N_\circ^{n,k}$	$k=0$	$k=1$	$k=2$	
$n=0$	1			$\leftarrow$ midpoint rule
$n=1$	$1/2$	$1/2$		
$n=2$	$2/3$	$-1/3$	$2/3$	

Newton–Cotes formulas

Thm. 126. A quadrature rule based on $n+1$ nodes is exact for P_n iff it is an interpolation quadrature formula.

Proof. $\Leftarrow$ Trivial.
$\Rightarrow$ It must be exact for all characteristic Lagrange polynomials $l_j(x)$. That is

$$\int_a^b l_k(x)\,\mathrm{d}x = \sum_{j=0}^{n} a_k l_k(x_j) = a_k. \blacksquare$$

Newton–Cotes formulas

Let $N^{n,k}$ denote the closed or the open Newton–Cotes coefficients.

Thm. 127.

$$\sum_{k=0}^{n} N^{n,k} = 1, \quad N^{n,k} = N^{n,n-k}.$$

Proof. In view of the previous theorem we have

$$\int_a^b 1 \, \mathrm{d}x = b - a = \sum_{k=0}^{n} (N^{n,k}(b-a)1) = (b-a) \sum_{k=0}^{n} N^{n,k}.$$

This proves the first statement. The second one follows from the symmetry $l_k(a+x) = l_{n-k}(b-x)$. ■

Rmk. If n is large then it is not practical to use the Newton–Cotes formulas. The Newton–Cotes coefficients $N^{n,k}$ may be negative that may cause cancellation. We generally use composite formulas.

Newton–Cotes formulas

Rmk. The Newton–Cotes formulas based on $n+1$ nodes are exact for P_n. If n is even, then they are exact also for P_{n+1}.

Namely, let p_{n+1} be a polynomial from P_{n+1}. Let us rewrite it to a polynomial of the term $(x-(a+b)/2)$.

$$p_{n+1}(x) = \alpha_{n+1}\left(x - \frac{a+b}{2}\right)^{n+1} + \underbrace{\alpha_n \left(x - \frac{a+b}{2}\right)^{n} + \ldots + \alpha_0}_{\text{The formula is exact for this.}},$$

moreover,

$$\int_a^b \underbrace{\alpha_{n+1}\left(x - \frac{a+b}{2}\right)^{n+1}}_{=:f(x)} \mathrm{d}x = (b-a)\sum_{k=0}^{n} \underbrace{N^{n,k}}_{N^{n,n-k}} \underbrace{f(x_k)}_{-f(x_{n-k})} = 0.$$

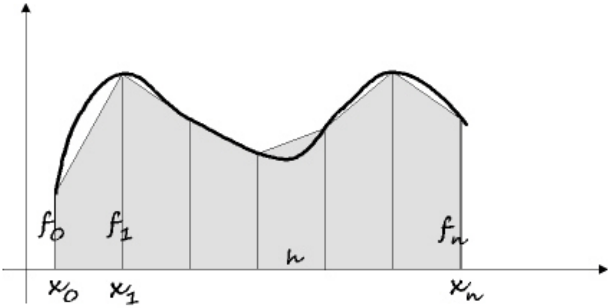
Thus the formula is exact for this polynomial.

Composite formulas

Composite trapezoidal rule

Let the nodes be equidistant with distance h. The so-calles composite trapezoidal rule approximates the integral as follows:

$$I_{\text{trap}}(f) = \frac{h}{2} f_0 + h \sum_{k=1}^{n-1} f_k + \frac{h}{2} f_n.$$



Composite trapezoidal rule

- Closed quadrature formula. The application of the formula is easy.
- $s_n \leq I_{\text{trap}}(f) \leq S_n$, that is, if the function is Riemann integrable, then the value of the formula tends to the exact integral value as the partition is refined.
- Order of exactness: 2. It is exact only on first degree polynomials. Order of the convergence is 2.

Example.

$$\int_0^1 \sin x/x \,\mathrm{d}x \approx 0.9460830704, \;\; n = 1/h.$$

n	$I_n(f)$	$\lvert I(f) - I_n(f)\rvert$
1	0.920735	0.25×10^{-1}
10	0.945832	0.25×10^{-3}
100	0.946080	0.25×10^{-5}
1000	0.9460830704	0.27×10^{-7}

Composite trapezoidal rule

Thm. 128. For $f \in C^2[a,b]$ functions, the error of the composite trapezoidal rule is

$$I(f) - I_{\text{trap}}(f) = -\frac{(b-a)h^2}{12} f^{(2)}(\eta),$$

where $\eta \in (a,b)$.

Rmk.

$$|I(f) - I_{\text{trap}}(f)| \leq \frac{(b-a)h^2}{12} M_2.$$

Lemma. (One of the mean value theorems of integral calculus.) If ϕ is a nonnegative integrable function on $[a,b]$ and g is continuous, then there exists a value $\eta \in (a,b)$ such that

$$\int_a^b \phi(x) g(x) \, \mathrm{d}x = g(\eta) \int_a^b \phi(x) \, \mathrm{d}x.$$

Composite trapezoidal rule

Proof. We use the error formula of the interpolation error and the above mean value theorem. Consider first the kth subinterval

$$\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x - \frac{f_k + f_{k-1}}{2}h$$

$$= \int_{x_{k-1}}^{x_k} \frac{f^{(2)}(\xi_x)(x - x_{k-1})(x - x_k)}{2}\,\mathrm{d}x$$

$$= -f^{(2)}(\eta_k)\int_{x_{k-1}}^{x_k} \frac{(x - x_{k-1})(x_k - x)}{2}\,\mathrm{d}x =$$

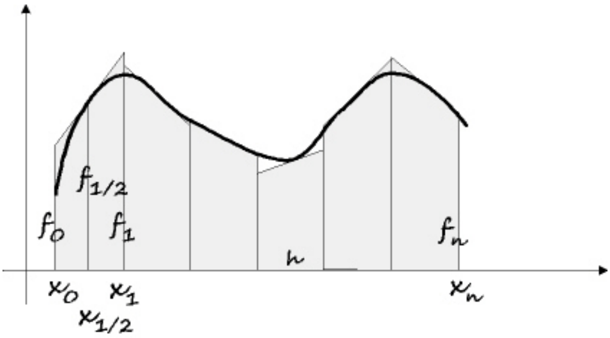
$$= -f^{(2)}(\eta_k)\frac{h^3}{12}.$$

Because we have n intervals, the total error has the form

$$-\sum_{k=1}^{n} f^{(2)}(\eta_k)\frac{h^3}{12} = -nf^{(2)}(\eta)\frac{h^3}{12} = -\frac{(b-a)h^2}{12}f^{(2)}(\eta)$$

with a suitably chosen $\eta \in (a, b)$ value. ■

Composite midpoint rule



$$I_{\mathsf{mid}}(f) = h(f_{1/2} + \ldots + f_{n-1/2}).$$

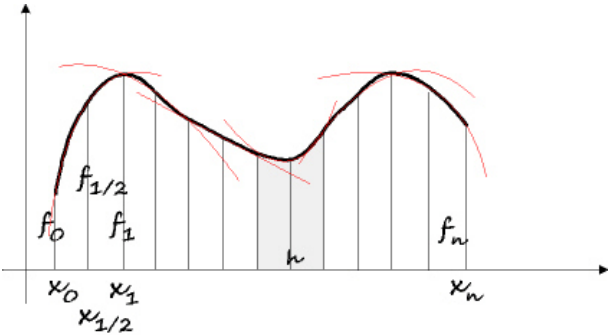
Open quadrature formula. Order: 2 (convergence and exactness).

Thm. 129. The error of the composite midpoint rule for $f \in C^2[a,b]$ functions is

$$I(f) - I_{\text{érintő}}(f) = \frac{(b-a)h^2}{24} f^{(2)}(\eta),$$

where $\eta \in (a,b)$.

Composite Simpson's rule



$$I_{\mathsf{Simp}}(f) = \frac{h}{6}(f_0 + 4f_{1/2} + 2f_1 + 4f_{3/2} + 2f_2 + \ldots + 4f_{n-1/2} + f_n).$$

Closed quadrature formula. Order: 4 (convergence and exactness).

Composite Simpson's rula

Thm. 130. The error of the composite Simpson's rule for functions $f \in C^4[a,b]$ is

$$I(f) - I_{\mathrm{Simp}}(f) = -\frac{(b-a)h^4}{2880} f^{(4)}(\eta),$$

where $\eta \in (a,b)$.

Rmk. In the case of a given partition:

$$I_{\mathsf{Simp}}(f) = \frac{I_{\mathsf{trap}}(f) + 2I_{\mathsf{mid}}(f)}{3}.$$

Rmk. All the above quadrature formulas tend to the exact integral for Riemann integrable functions as $h \to 0$.

Gaussian quadrature

Gaussian quadrature

We have used equidistant nodes so far. We have seen, however, that these set of nodes are not efficient in interpolation problems.
We are looking for a better solution.

$$I_s(f) := \int_a^b s(x)f(x)\,\mathrm{d}x \approx \sum_{k=0}^{n} a_k f_k =: I_{n,s}(f),$$

where $a \leq x_0 < x_1 < \ldots < x_n \leq b$ are arbitrary nodes and s is a positive weight function.

If the quadrature formula is an interpolation quadrature formula, then we have

$$a_k = \int_a^b s(x)l_k(x)\,\mathrm{d}x$$

and the quadrature formula is exact for P_n.

How to choose the nodes to make the order of the exactness as large as possible?

Gaussian quadrature

Thm. 131. The interpolation quadrature formula

$$I_{n,s}(f) = \sum_{k=0}^{n} a_k f_k$$

is exact for P_{n+m} if and only if

$$\int_a^b w_{n+1}(x) s(x) p(x) \, \mathrm{d}x = 0$$

for all $p \in P_{m-1}$.

Rmk. The formula cannot be exact for P_{2n+2}. To see this, let us take $p = w_{n+1}$. From the inequality

$$\int_a^b s(x) w_{n+1}^2(x) \, \mathrm{d}x = 0$$

we have $w_{n+1} \equiv 0$, which shows a contradiction.

Gaussian quadrature

Def. 132. Let $f, g \in C[a, b]$. We call these functions orthogonal on the interval $[a, b]$ with respect to the positive weight function s, if

$$\int_a^b s(x)f(x)g(x)\,\mathrm{d}x = 0.$$

Thm. 133. Let us suppose that the polynomials $p_0, p_1, \ldots$ (the subscript denotes the degree of the polynomial) are pairwise orthogonal on $[a, b]$ with respect to the weight function s. Then all the zeros of these polynomials are real, single and lie in the interval $[a, b]$.

Construction of the Gaussian quadrature formulas: We orthogonalize the polynomials $1, x, \ldots$ with respect to the weight function: $p_0, p_1, \ldots$. We define the zeros of these polynomials $(x_0, \ldots, x_n)$ to be the nodes of the quadrature formula. We calculate the quadrature weights as $a_k = \int_a^b s(x)l_k(x)\,\mathrm{d}x$.
Then the form of the quadrature formula is

$$I_{n,s}(f) = \sum_{k=0}^{n} a_k f(x_k).$$

Gaussian quadrature

Legendre polynomials ($s(x) = 1$, $[-1, 1]$): $p_0 = 1$, $p_1 = x$, $p_2 = x^2 - 1/3$, etc.

Chebishev polynomials ($s(x) = 1/\sqrt{1 - x^2}$, $[-1, 1]$): $p_0 = 1$, $p_1 = x$, $p_2 = x^2 - 1/2$, $p_3 = x^3 - 3x/4$ etc.

Example. Let us construct the three-point Gauss–Chebyshev quadrature formula! The zeros of p_3 are 0 and $\pm\sqrt{3}/2$. These are the nodes. The weights

$$a_0 = \int_{-1}^{1} \frac{x(x - \sqrt{3}/2)}{-\sqrt{3}/2(-\sqrt{3}/2 - \sqrt{3}/2)} \frac{1}{\sqrt{1 - x^2}} \, \mathrm{d}x = \pi/3,$$

similarly $a_1 = a_2 = \pi/3$. Thus the formula is:

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, \mathrm{d}x \approx \frac{\pi}{3}(f(-\sqrt{3}/2) + f(0) + f(\sqrt{3}/2)).$$

Gaussian quadrature

Some nodes and weights of Gaussian quadrature.

	Gauss–Legendre		Gauss–Chebyshev	
	$s(x) = 1$		$s(x) = 1/\sqrt{1-x^2}$	
Nr. of points	Nodes	Weights	Nodes	Weights
1	0	2	0	π
2	$\frac{-1}{\sqrt{3}}, \frac{1}{\sqrt{3}}$	1,1	$\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$	$\frac{\pi}{2}, \frac{\pi}{2}$
3	$-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}$	$\frac{5}{9}, \frac{8}{9}, \frac{5}{9}$	$\frac{-\sqrt{3}}{2}, 0, \frac{\sqrt{3}}{2}$	$\frac{\pi}{3}, \frac{\pi}{3}, \frac{\pi}{3}$