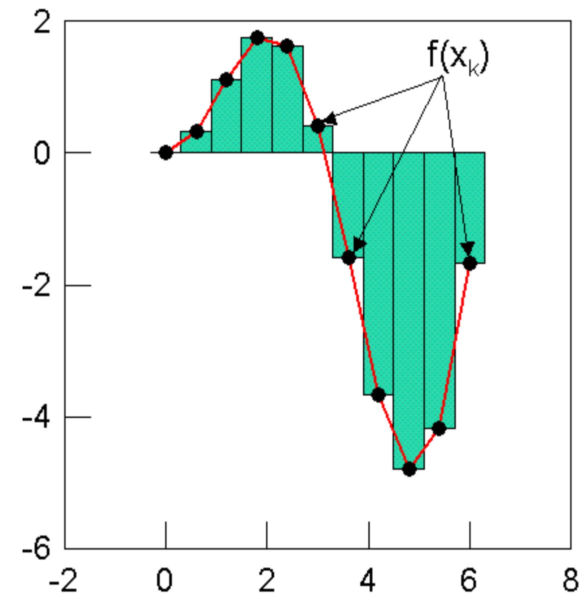
Numerical integration of functions

outline

- general formulation of integral quadrature
- closed Newton-Cotes formulas
- open Gauss-type quadratures
- multidimensional integrals

Numerical integration

Numerical integration is one of the common tasks in scientific computation. We know of only several types of integrals that can be computed analytically, in all the others cases the value of integral must be estimated numerically with required accuracy.



Thus we may pose a problem, how to estimate the value of definite integral

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

The straightforward solution is to replace the integrand function f(x) with interpolation polynomial, we just need a sequence of nodes and corresponding functions values

$$\{(x_0, y_0),\ (x_1, y_1),\ (x_2, y_2),\ \ldots,\ (x_N, y_N)\}$$

Integration of polynomials is straightforward

$$\varphi(x) = \sum_{k=0}^{N} \Phi_k(x)\, f(x_k), \quad \Phi_k(x) - \text{Lagrange's nodal polynomials}$$

$$\int_a^b f(x)dx \approx \int_a^b \varphi(x)dx = \sum_{k=0}^{N} f(x_k) \int_a^b \varphi_k(x)dx = \sum_{k=0}^{N} f(x_k) A_k$$

$$S = \sum_{k=0}^{N} A_k f(x_k)$$

← this formula defines the quadrature
A_k are the weights to be defined

Closed Newton-Cotes quadratures

We consider the proper intergals, i.e. the boundaries are finite and the integrand has no singularities within integration interval

$$C = \int_a^b f(x)dx, \qquad |a|, |b| < \infty, \bigwedge_{x\in[a,b]} |f(x)| < \infty$$

We define a sequence of equidistant nodes. In Newton-Cotes quadratures the first and the last nodes coincide with integration boundary points a and b

$$h = \frac{b-a}{N}$$
$$x_k = a + h \cdot k, \quad k = 0, 1, 2, \ldots, N$$
$$f(x_k) \equiv f_k$$

To accomplish numerical integration the coefficients of quadrature need to be known, these we get from the direct integration of nodal polynomials

$$A_k = \int_a^b \Phi_k(x)dx \qquad \Phi_k(x) = \prod_{\substack{j=0 \\ j\neq k}} \frac{x - x_j}{x_k - x_j}$$

To make further integration easier let's transform the the integration variable into unitless one

$$x \in [a, b] \implies t \in [0, N]$$

$$x = a + ht \quad \rightarrow \quad \frac{x - x_j}{x_k - x_j} = \frac{a + ht - a - hj}{a + hk - a - hj} = \frac{t - j}{k - j} \quad \rightarrow \quad \Phi_k(t) = \prod_{\substack{j=0 \\ j\neq k}} \frac{t - j}{k - j}$$

Now let's rewrite explicitly the nodal polynomial for the new variable

$$\Phi_k(t) = \prod_{\substack{j=0 \\ j\neq k}} \frac{t-j}{k-j}$$

$$= \frac{(t-0)(t-1)\dots(t-[k-1])\cdot(t-[k+1])\dots(t-N)}{(k-0)(k-1)\dots(k-[k-1])\cdot(k-[k+1])\dots(k-N)}$$

$$= \frac{(t-0)(t-1)\dots(t-[k-1])\cdot(t-[k+1])\dots(t-N)}{(1\cdot 2\cdot\ldots\cdot k)\cdot(-1)\cdot(-2)\cdot\ldots\cdot(-[N-k])}$$

$$= \frac{(t-0)(t-1)\dots(t-[k-1])\cdot(t-[k+1])\dots(t-N)}{k!(-1)^{N-k}(N-k)!}$$

fill this empty site multiplying by factor

$$\frac{t-k}{t-k}$$

$$= \frac{(-1)^{N-k}}{k!(N-k)!}\frac{t(t-1)\dots(t-N)}{(t-k)}$$

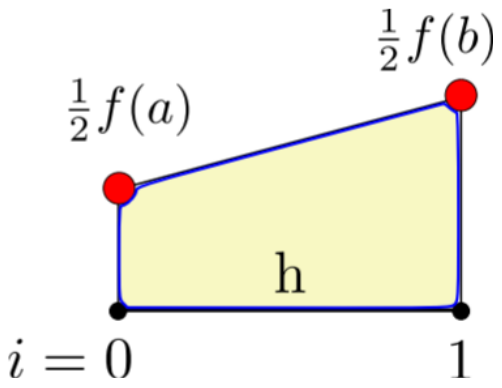
We get more compact expression, ready to put into integral, which is directly used in calculations of weights A_k

$$A_k = \int_0^N \Phi_k(t)\,dt = h\frac{(-1)^{N-k}}{k!(N-k)!}\int_0^N \frac{t(t-1)\dots(t-N)}{(t-k)}dt$$

Trapezoidal formula

The simplest quadrature is defined for two nodes (N=1)
it is called **trapezoidal formula**

$$A_k = h\frac{(-1)^{N-k}}{k!(N-k)!}\int_0^N \frac{t(t-1)\dots(t-N)}{(t-k)}dt$$



$$A_0 = -h\int_0^1 (t-1)dt = \frac{1}{2}h$$

$$A_1 = h\int_0^1 t dt = \frac{1}{2}h$$

$$h = b - a \qquad S(f) = \frac{1}{2}h(f_0 + f_1)$$

- interplation for two nodes is exact for linear function, and this class of functions can be integrated exactly
- to obtain the estimation of the integration error we shall integrate an interpolation error

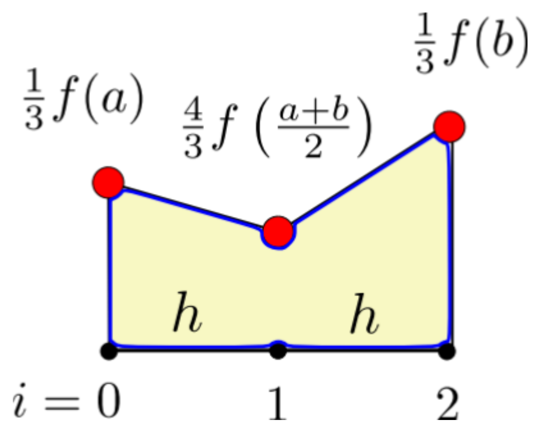
$$R_{N+1}(x) = f(x) - L_N(x) = \frac{1}{(N+1)!}\omega_{N+1}(x)f^{(N+1)}(\xi), \qquad \xi \in (a,b)$$

$$E(f) = \frac{1}{2!}\int_a^b (x-a)(x-b)f^{(2)}(\xi)dx = -\frac{1}{12}h^3 f^{(2)}(\xi), \quad \xi \in [a,b]$$

Simpson formula

The next formula we get for three nodes (N=2), it is called **Simpson formula**, it excatly integrates the quadratic function

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



$$A_0 = \frac{1}{3}h \qquad A_1 = \frac{4}{3}h \qquad A_2 = \frac{1}{3}h$$

$$S(f) = \frac{1}{3}h(f_0 + 4f_1 + f_2)$$

- calculating the error in standard way we encounter **Simpson paradox**, due to symmetry of integral interval the integration error vanishes (odd parity function integrated over symmetric interval gives zero) what can not be the truth

$$E(f) \sim \int_a^b (x-a)\left(x - \frac{a+b}{2}\right)(x-b)dx = 0$$

- therefore we add one more fictious point which is shifted towards the central node, hence the Simpson quadrature is one more order higher than it results from its constructon

$$E(f) = \frac{f^{(4)}(\xi_1)}{4!}\int_a^b (x-a)\left(x - \frac{a+b}{2}\right)^2 (x-b)dx = -\frac{1}{90}h^5 f^{(4)}(\xi), \quad \xi \in [a,b]$$

Coefficients of commonly used integration quadratures

N	w	A_0/w	A_1/w	A_2/w	A_3/w	A_4/w	A_5/w	A_6/w	error	name
1	(1/2)h	1	1						h^3 (1/12) $f^{(2)}(\xi)$	trapezoidal
2	**(1/3)h**	**1**	**4**	**1**					h^5 **(1/90)** $f^{(4)}(\xi)$	**SImpson**
3	(3/8)h	1	3	3	1				h^5 (3/80) $f^{(4)}(\xi)$	3/8
4	**(4/90)h**	**7**	**32**	**12**	**32**	**7**			h^7 **(8/945)** $f^{(6)}(\xi)$	**Milne**
5	(5/288)h	19	75	50	50	75	19		h^7 (275/12096) $f^{(6)}(\xi)$	-------
6	(6/840)h	41	216	27	272	27	216	41	h^9 (9/1400) $f^{(8)}(\xi)$	Weddle

Compsite integration formulas

- since the lecture concerning the polynomial interpolation we know that the use of high degree polynomials for homogeneously distributed nodes has no any sense due to the Runge effect
- instead, integration interval is divided into segments and integration is performed within each segment with low order quadrature, partial results are summed giving hence the **composite formulas**

Trapezoidal composite formula

- integration interval is divided into n subintervals of equal length, each segment contains two nodes

$$x \in [a,b], \quad h = \frac{b-a}{n}, \quad x_k = a + h \cdot k, \quad f(x_k) = f_k, \qquad k = 0,1,2,\ldots,n$$

$$S(f) = \sum_{k=0}^{n-1} \frac{1}{2} h (f_k + f_{k+1}) = h\left(\frac{1}{2} f_0 + f_1 + \ldots + f_{n-1} + \frac{1}{2} f_n\right)$$

- subinterval integration errors are summed giving estimation of total error

$$E(f) = -\frac{h^3}{12}\sum_{k=0}^{n-1} f^{(2)}(\xi_k) = -\frac{(b-a)^3}{12n^2} \cdot \underbrace{\frac{1}{n}\sum_{k=0}^{n-1} f^{(2)}(\xi_k)}_{f^{(2)}(\xi),\, \xi\in[a,b]} \qquad \xi_k \in (a+kh, a+(k+1)h)$$

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

- to make the estimation of integral more accurate we need to increase the number of integration nodes

Composite Simpson formula

- integration interval is divided into m/2 subintervals, m - must be even, integration is made for three nodes in each subinterval and the partial results are summed up

$$x \in [a,b], \quad h = \frac{b-a}{n}, \quad x_k = a + h \cdot k, \quad f(x_k) = f_k, \qquad k = 0,1,2,\ldots,n$$

$$S(f) = \frac{h}{3}\sum_{k=1}^{n/2}(f_{2k-2} + 4f_{2k-1} + f_{2k})$$

$$= \frac{h}{3}\left[f_0 + f_n + \underbrace{2(f_2 + f_4 + \ldots + f_{n-2})}_{\text{even indices}} + \underbrace{4(f_1 + f_3 + \ldots + f_{n-1})}_{\text{odd indices}}\right]$$

- error of integration

$$E(f) = -\frac{h^5}{90}\sum_{k=1}^{n/2} f^{(4)}(\xi_k) = -\frac{h^5}{90}\frac{n}{2}\left(\frac{2}{n}\sum_{k=1}^{n/2} f^{(4)}(\xi_k)\right)$$

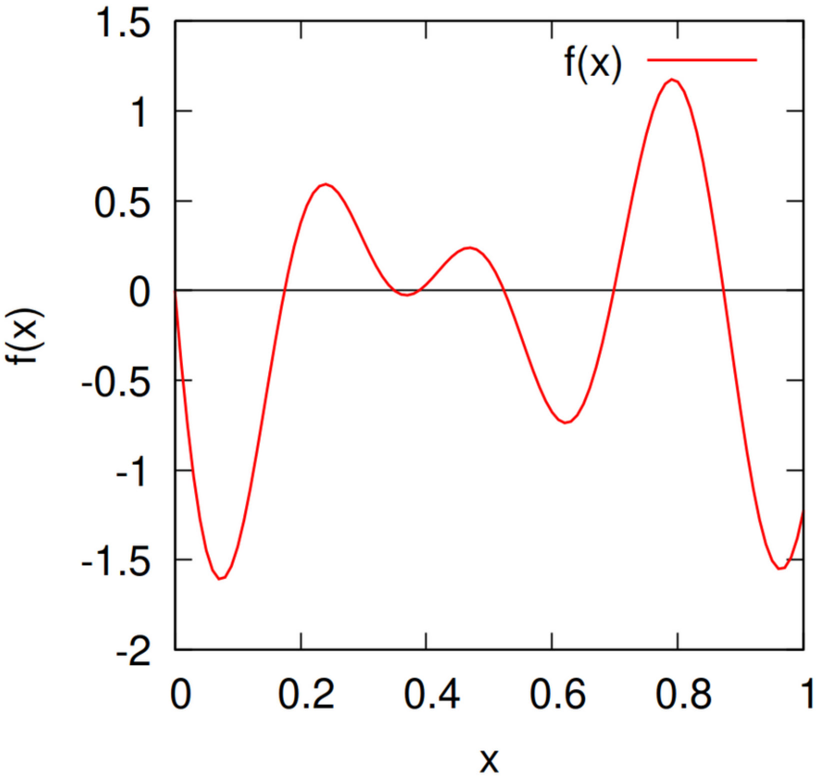
$$E(f) = -\frac{(b-a)^5}{180\, n^4} f^{(4)}(\xi)$$

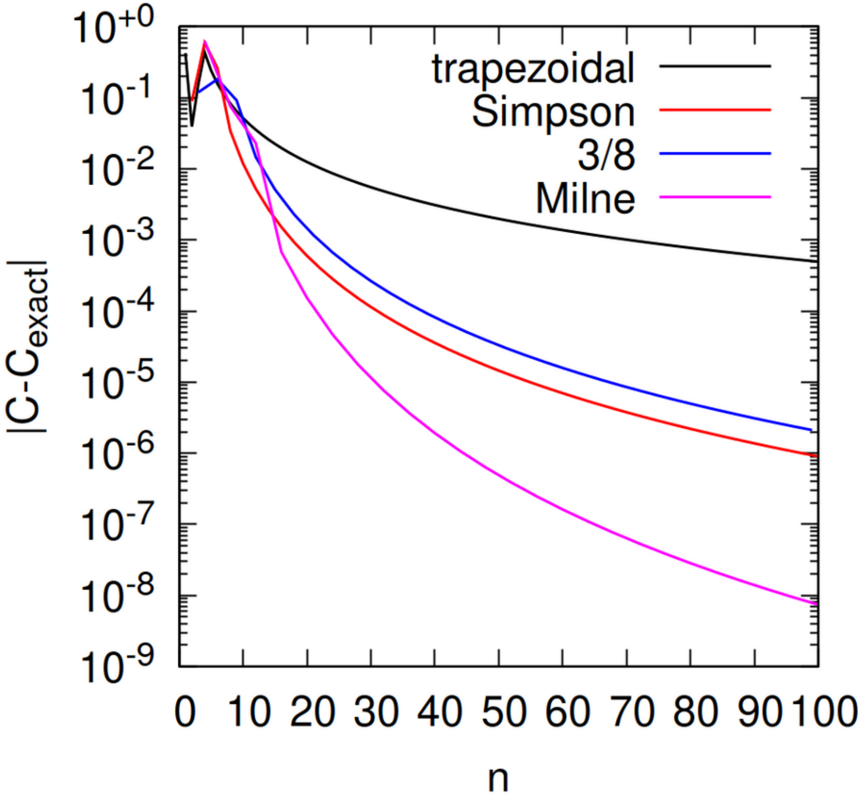
- error decreases much faster for larger m than for trapezoidal formula

Example: numerical integration by means of few low-order quadratures

$$f(x) = \log\left(x^3 + 3x^2 + x + 0.1\right) \cdot \sin(18x)$$

$$C = \int_0^1 f(x)dx = ?$$





Richardson extrapolation

Let's consider the composite trapezoidal formula for **n** and **2n** nodes

$$n \quad \Longrightarrow \quad C_n, \quad E_n(f) = -\frac{(b-a)^3}{12 \cdot n^2} f^{(2)}(\xi)$$

$$2n \quad \Longrightarrow \quad C_{2n}, \quad E_{2n}(f) = -\frac{(b-a)^3}{12 \cdot 4 \cdot n^2} f^{(2)}(\xi)$$

we recognize simple relation between both errors

$$4\, E_{2n}(f) = E_n(f)$$

this suggests both integral estimations might help in decreasing the integration error by at least one order

$$\widetilde{C} = \frac{4 \cdot C_{2n} - 1 \cdot C_n}{4 - 1}$$

$$\widetilde{E}(f) = \frac{4 \cdot E_{2n} - E_n}{4 - 1} \leq O\left(\frac{1}{n^3}\right)$$

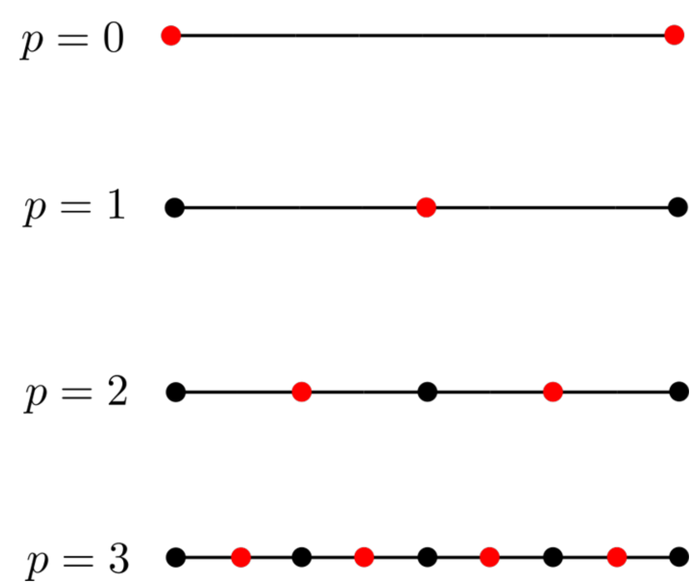
- coefficients in numerator are chosen so as to cancel leading term in error formula
- coefficients in denumerator are just copies of these from numerator and are used to normalize the result

Romberg integration method

- it uses the conclusions from Richardson extrapolation, by iteratively doubling the number of nodes in composite trapezoidal formale we get the better results, but these are further improved by cancellation of leading error terms

- by first we define the positions of equdistant nodes with the length of single segment depending on the number p which enumerates consecutive doubling of nodes

$$h_p = \frac{b-a}{2^p}$$



- at start, the method uses only two nodes p=0

$$R_{0,0} = \frac{1}{2}(b-a)\left[f(a) + f(b)\right]$$

- next we calculate the more accurate results doubling the number of nodes, but calculating the new estimation the previous one is reused and only the new added nodes need to be iterated

$$R_{p,0} = \underbrace{\frac{1}{2}R_{p-1,0}}_{\text{old nodes}} + \underbrace{\frac{b-a}{2^p}\sum_{i=1}^{2^{p-1}} f\left(a + (2i-1)\frac{b-a}{2^p}\right)}_{\text{new nodes}}$$

- having two first integral estimations we may start to improve the results

$$R_{p,m} = \frac{4^m R_{p,m-1} - R_{p-1,m-1}}{4^m - 1}$$

$$\begin{array}{lllll} R_{0,0} & & & \textbf{better} \longrightarrow & \\ R_{1,0} & R_{1,1} & & & \\ R_{2,0} & R_{2,1} & R_{2,2} & & \\ \vdots & \vdots & \vdots & \ddots & \\ R_{p,0} & R_{p,1} & R_{p,2} & \dots & R_{p,p} \end{array}$$

Example: numerical integration with composite trapezoidal formula and Romberg method

$$f(x) = ln\left(x^3 + 3x^2 + x + 0.1\right) \cdot \sin(18x)$$

$$C = \int_0^1 f(x)dx = ?$$

n	$R_{p,0}$	$R_{p,p}$
2	-0.6117694	-0.6117694
3	-0.2257981	-0.0971410
5	0.2498394	0.4420869
9	-0.1032663	-0.2741157
17	-0.1668214	-0.1842338
33	-0.1816364	-0.1864996
65	-0.1852783	-0.1864869
129	-0.1861850	-0.1864869
257	-0.1864114	-0.1864869
513	-0.1864680	-0.1864869
1025	-0.1864822	-0.1864869
2049	-0.1864857	-0.1864869
4097	-0.1864866	-0.1864869
8193	-0.1864868	-0.1864869
16385	-0.1864869	-0.1864869
32769	-0.1864869	-0.1864869

convergence for 2^7 nodes

convergence for 2^{15} nodes

Gauss quadrature

Many integrals are not well behaved as we yet considered, much problems extends over infinite length region, and singularities might occur in the integrands especially at the ends of the integral interval, despite this fact the intergral may have finite value.

$$\int_0^1 \frac{\sin(x)}{x^{\frac{1}{2}}} dx \approx 0.6205366026$$

To cope with such problems we change the beggining assumption concerning the nodes' position: now we assume these might be distributed unevenly over the interval, this gives us additional N+1 free parameters besides the N+1 quadrature coefficients A_k. The order of Gauss quadrature is about twice the order of Newton-Cotes ones – 2N instead of N.

Since we want also to cope with integrand's singularities we put in the integral a weighting function w(x) while the integrand function f(x) will be interpolated by **orthogonal polynomials**

$$C = \int_a^b w(x) f(x) dx$$

$$P = \{p_0(x), p_1(x), p_2(x) \ldots, \} \quad \Longrightarrow \quad \int_a^b w(x) p_k(x) p_m(x) dx = \delta_{k,m}$$

$$f(x) = \sum_{k=1}^{N} f(x_k)\, p_k(x)$$

$$A_k = \int_a^b w(x) p_k(x)$$

The general formula for weights A_k ,i.e. irrespectie of the type of polynomials, was derived from Christoffel-Darboux identity

$$A_k = -\frac{\beta_{N+1}\gamma_N}{\beta_N p_{N+1}(d_k) p'_N(d_k)} \quad k = 1, 2, \ldots, N$$

$$\gamma_n = \int_a^b w(x) p_k^2(x) dx$$

d_k - k-th zero of $p_N(x)$

β_N, β_{N+1} - multipliers of leading monomials in $p_N(x)$ and $p_{N+1}(x)$

Currently the weights A_k and the nodes x_k (d_k) are commonly calculated by Golub-Welsch diagonalization method.

The recurrence formula for generating the sequence of orthogonal polynomials is rewritten as standard eigenvalue problem, the eigenvalues are the nodes while the first entries in the eigenvectors are integration weights A_k.

Finding nodes and weights with Golub-Welsch method

We form the tridiagonal symmetric matrix

$$J = \begin{bmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \sqrt{b_2} & \ddots & \ddots & \\ & & \ddots & a_{n-2} & \sqrt{b_{n-2}} \\ & & & \sqrt{b_{n-2}} & a_{n-1} \end{bmatrix}$$

and solve this eigenvalue problem

$$J\vec{v}_k = \lambda_k \vec{v}_k$$

eigenvalues are the nodes

$$x_k = \lambda_k, \quad k = 0, 1, \ldots, n-1$$

while the weights we get from the first entries of eigenvectors

$$w_k = \mu \cdot v_{k,0}^2$$

$$\mu = \int_a^b w(x)dx$$

- Gauss-Legendre

$$a_i = 0, \quad b_i = \frac{1}{4 - \frac{1}{i^2}}, \quad \mu = 2$$

- Gauss-Laguerre

$$a_i = 2 \cdot i + 1, \quad b_i = i^2, \quad \mu = 1$$

- Gauss-Hermite

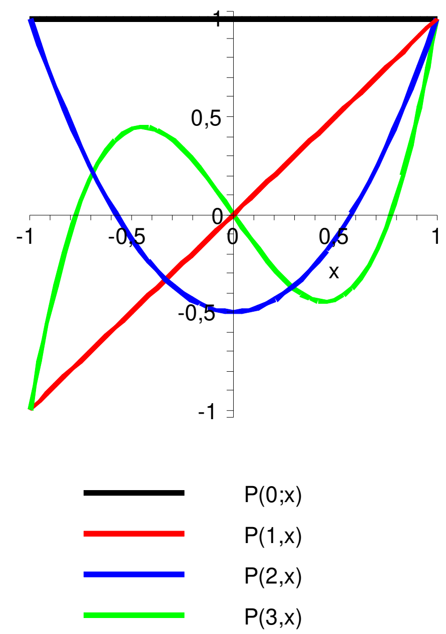
$$a_i = 0, \quad b_i = \frac{i}{2}, \quad \mu = \sqrt{\pi}$$

Gauss-Legendre quadrature

$$x \in [-1, 1], \quad w(x) = 1,$$

$$C = \int_{-1}^{1} f(x)\, dx$$

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$$



- scaling the interval of integration

$$t \in [a, b] \quad \Longrightarrow \quad t = \frac{a+b}{2} + \frac{b-a}{2}x \quad \Longrightarrow \quad f\left(\frac{a+b}{2} + \frac{b-a}{2}x\right) = g(x)$$

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

$$\int_a^b f(t)dt \approx S(f) = \frac{b-a}{2}\sum_{k=1}^{N} A_k f(t_k) \qquad t_k = \frac{a+b}{2} + \frac{b-a}{2}x_k$$

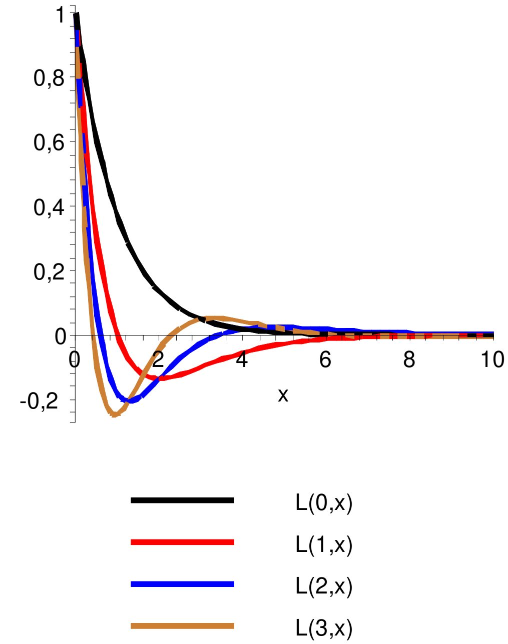
Remark: usually the routine we use for calculations of A_k and x_k, automatically scales both factors

Gaus-Laguerre quadrature

$$x \in [0, \infty), \quad w(x) = e^{-x}$$

$$C = \int_0^\infty f(x)\, e^{-x}\, dx$$

$$(n+1)L_{n+1} = (2n+1-x)L_n - nL_{n-1}$$

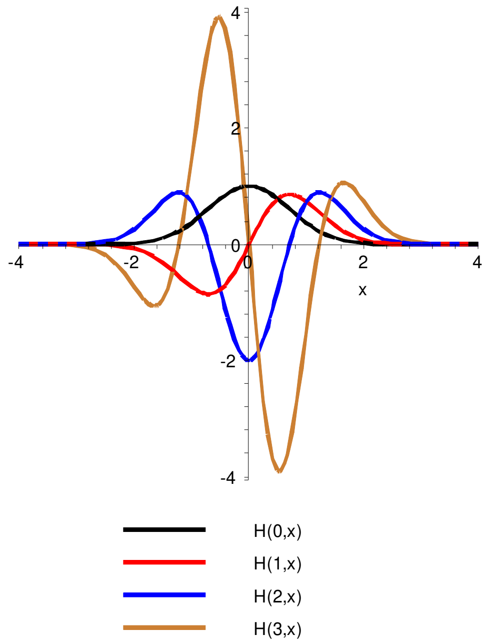


Gauss-Hermite quadrature

$$x \in (-\infty, \infty), \quad w(x) = e^{-x^2}$$

$$C = \int_\infty^\infty f(x)\, e^{-x^2}\, dx$$

$$H_{n+1} = 2xH_n - 2nH_{n-1}$$



Example: calculation of improper integral with Gauss quadrature

$$C = \int_0^\infty \log(x) e^{-x^2} dx = -0.8700577$$

- Gauss-Legendre

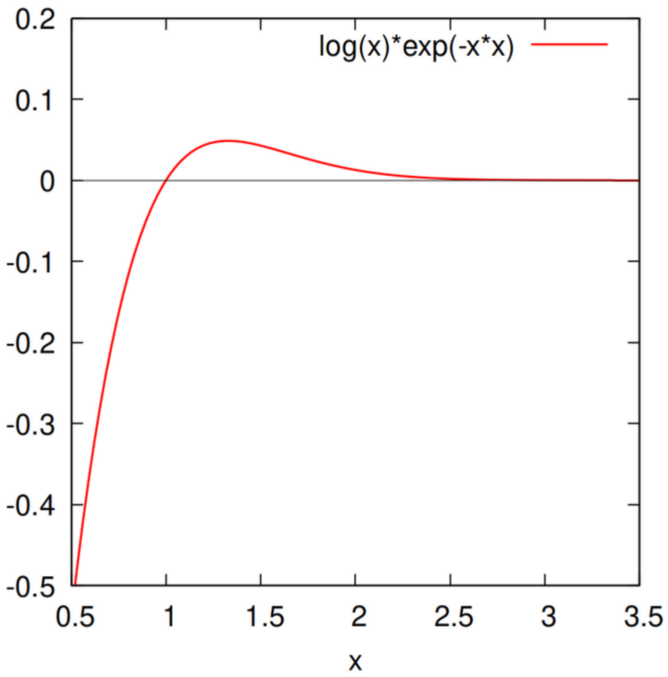
$$C = \int_0^{3.5} \underbrace{\log(x)\, e^{-x^2}}_{f(x)} dx$$

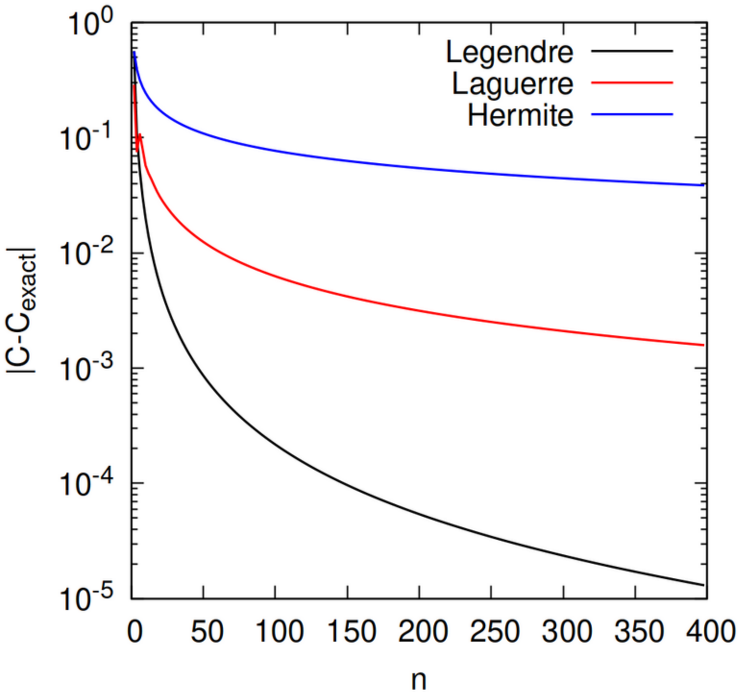
- Gauss-Laguerre

$$C = \int_0^\infty \underbrace{\frac{\log(x) e^{-x^2}}{e^{-x}}}_{f(x)} \underbrace{e^{-x}}_{w(x)} dx$$

- Gauss-Hermite

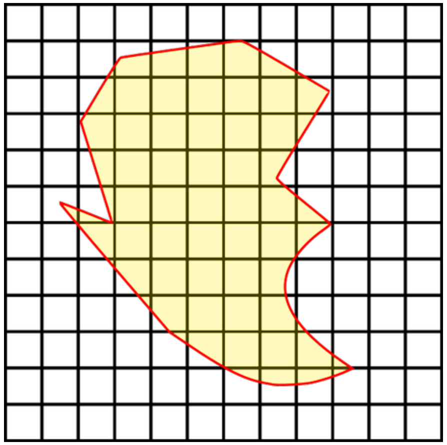
$$C = \int_{-\infty}^\infty \underbrace{\frac{1}{2}\log|x|}_{f(x)} \underbrace{e^{-x^2}}_{w(x)} dx$$





Multidimensional integrals

- in one dimensional probelms we can easily interpolate the integrand with polynomial, but it couldn't be an easy task for even two-dimensional problem with irregular boundaries
- the boundaries' shapes are crucial since the curvature may change locally quite fast making an automatic integration difficult
- generally, the numerical integration of multidimensional function utilizes the linearity of integration and relies on composition of sequence of M one-dimensional quadratures



$$\Omega \subset R^M$$

$$a_1 \le x_1 \le b_1$$
$$a_2(x_1) \le x_2 \le b_2(x_1)$$
$$\dots\dots\dots\dots\dots\dots\dots\dots$$
$$a_M(x_1, x_1, \dots, x_{M-1}) \le x_M \le b_M(x_1, x_2, \dots, x_{M-1})$$

$$C(f) = \underbrace{\int \dots \int}_{\Omega} f(x_1, x_2, \dots, x_M) dx_1 \dots dx_M$$

$$= \sum_{i_1=0}^{n_1} \sum_{i_2=0}^{n_2} \dots \sum_{i_M=0}^{n_M} A_{i_1} A_{i_2} \dots A_{i_M} f(x_{i_1}, x_{i_2}, \dots, x_{i_M},)$$

Remark: composition of one-dimensional quadratures may work properly for up to 4-6 dimensions, the higher-dimensional integrals can be estimated only with Monte Carlo method.