Numerical Integration

Why Numerical Integrations?

- To evaluate the definite integral

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

- Fundamental theorem of calculus:

  If there exists a function $F(x)$ such that $F'(x) = f(x)$

  then $$I = \int_a^b f(x)\,dx = F(b) - F(a)$$

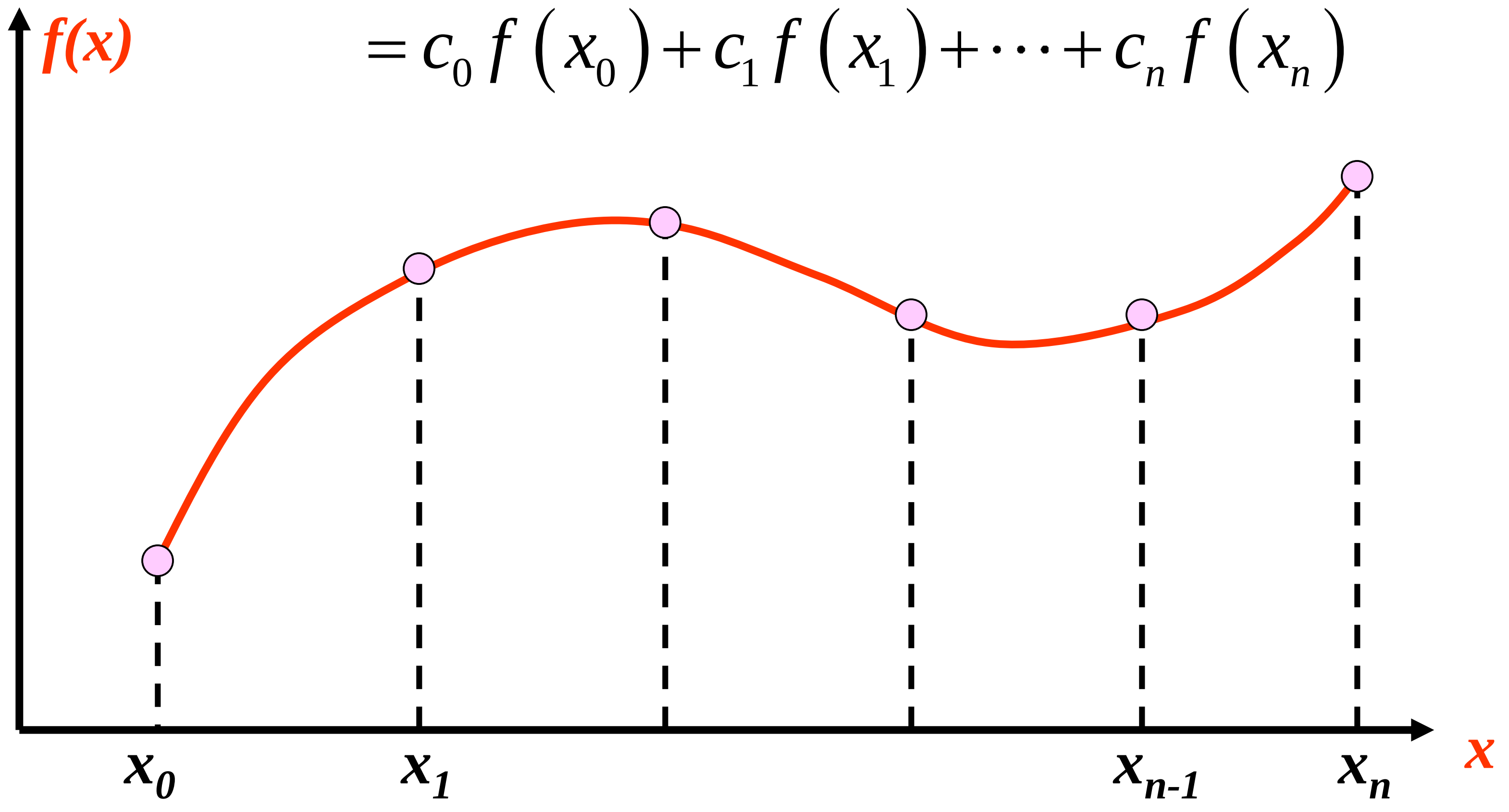
- In general, no analytic $F(x)$, have to evaluate the definite integral numerically.

Basic Idea

Weighted sum of function values

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

$$= c_0 f(x_0) + c_1 f(x_1) + \cdots + c_n f(x_n)$$



We denote that

$$I(a,b) = \int_a^b f(x)dx$$

The Trapezoidal Rule

We divide the interval from a to b into N slices. Each slide has width $h = (b-a)/N$.

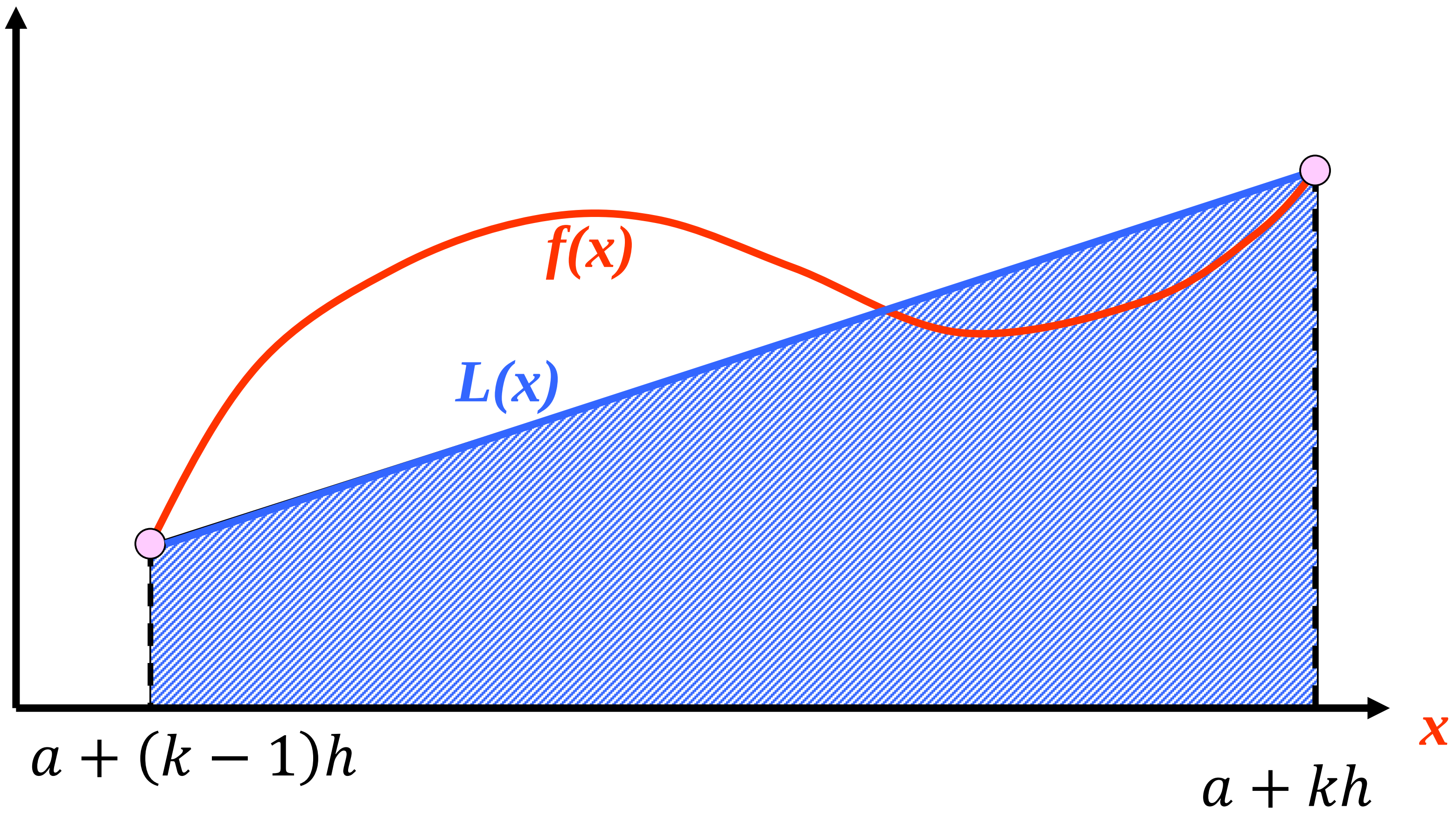
The area of k th slice is

$$A_k = \frac{1}{2}h[f(a+(k-1)h) + f(a+kh)].$$

$$\therefore \; I(a,b) \simeq \sum_{k=1}^{N} A_k = h\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right]$$

Trapezoidal Rule

Straight-line approximation



Simpson's Rule (quadratic curve)

We divide the interval from a to b into N slices. We fit a quadratic curve in each slice by using its midpoint and two endpoints.

For instance, we fit a quadratic though $x = -h, 0, +h$. Then we have three equations:

$$f(-h) = Ah^2 - Bh + C\,, \qquad f(0) = C\,, \qquad f(h) = Ah^2 + Bh + C$$

The area of this slice is

$$\int_{-\mathrm{h}}^{\mathrm{h}} (Ax^2 + Bx + C)dx = \frac{1}{3}h[f(-h) + 4f(0) + f(h)]\,.$$

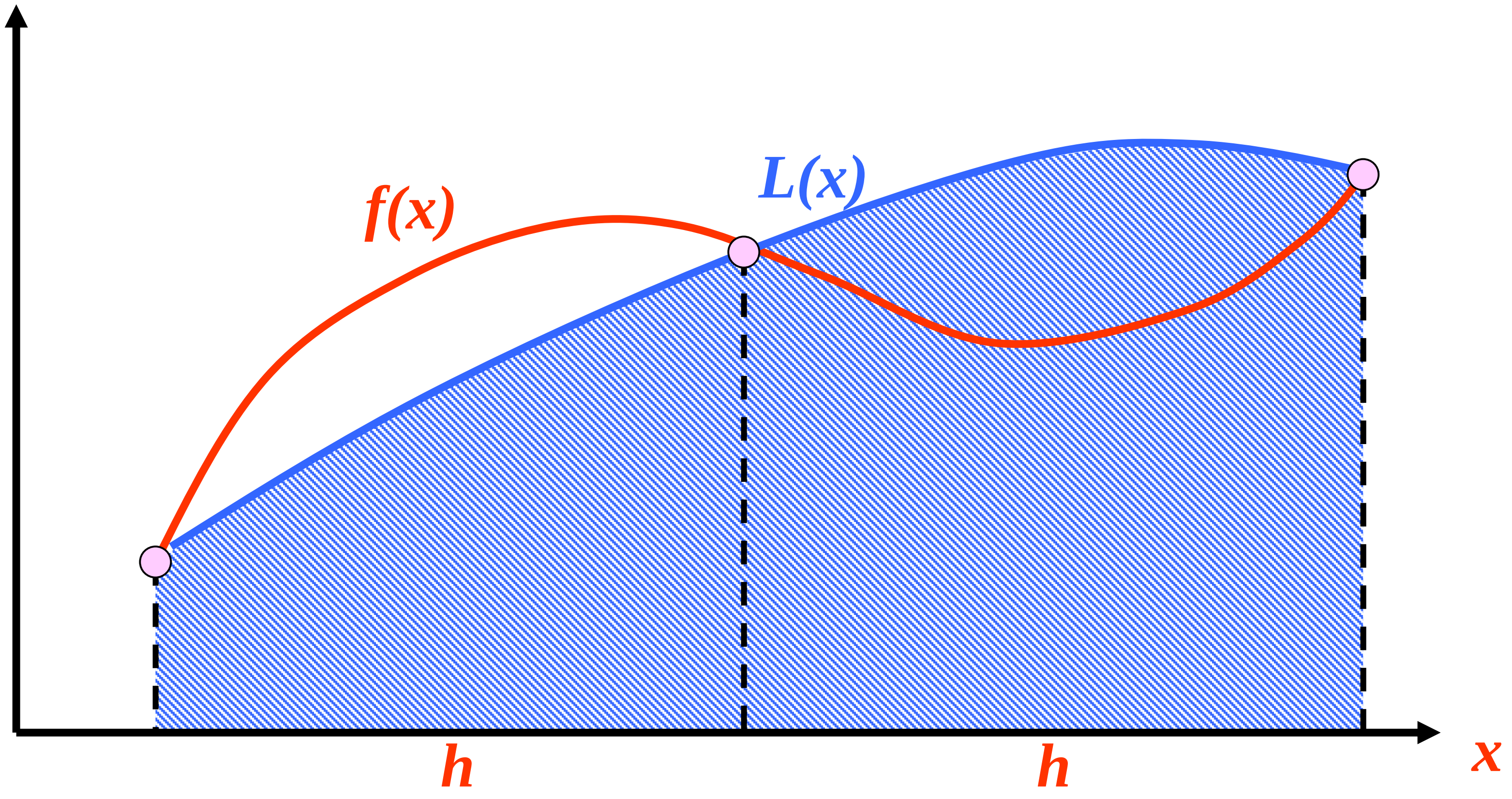
The total area under the quadratics is

$$I(a,b)$$
$$\simeq \frac{1}{3}h[f(a) + 4f(a+h) + f(a+2h)] + \frac{1}{3}h[f(a+2h) + 4f(a+3h) + f(a+4h)] + \cdots$$
$$+ \frac{1}{3}h[f(a+(N-2)h) + 4f(a+(N-1)h) + f(b)]$$

$$I(a,b) \simeq \frac{1}{3}h\left[f(a) + f(b) + 4\sum_{k=1}^{\frac{N}{2}} f(a+(2k-1)h) + 2\sum_{k=1}^{\frac{N}{2}-1} f(a+2kh)\right]$$

Simpson's Rule

Approximate the function by a parabola



Error of Integral

There are two main sources of error, i.e. Approximation error and rounding error.

Consider the trapezoidal rule:

Look at the slice fall between x_{k-1} and x_k.Perform Taylor expansions of $f(x)$ about $x_{k-1}$and x_k.

$$f(x) = f(x_{k-1}) + (x - x_{k-1})f'(x_{k-1}) + \frac{1}{2}(x - x_{k-1})^2 f''(x_{k-1}) + \cdots$$

$$f(x) = f(x_k) + (x - x_k)f'(x_k) + \frac{1}{2}(x - x_k)^2 f''(x_k) + \cdots$$

Integrating both expressions from x_{k-1} to x_k, and taking average,

$$\int_{x_{k-1}}^{x_k} f(x)dx = \frac{1}{2}h[f(x_{k-1}) + f(x_k)] + \frac{1}{4}h^2[f'(x_{k-1}) - f'(x_k)]$$

$$+ \frac{1}{12}h^3[f''(x_{k-1}) + f''(x_k)] + \frac{1}{48}h^4[f'''(x_{k-1}) - f'''(x_k)] + O(h^5)$$

Thus the full integral is

$$\int_a^b f(x)dx = \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} f(x)dx$$

$$= \frac{1}{2}h \sum_{k=1}^{N} [f(x_{k-1}) + f(x_k)] + \frac{1}{4}h^2[f'(a) - f'(b)] + \frac{1}{12}h^3 \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)]$$
$$+ \frac{1}{48}h^4[f'''(a) - f'''(b)] + O(h^4)$$

The error of the trapezoidal rule is

$$O(h^2) = \frac{1}{4}h^2[f'(a) - f'(b)] + \frac{1}{12}h^3 \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)] + O(h^4)$$

However,

$$\int_{\mathrm{a}}^{\mathrm{b}} f''(x)dx = \frac{1}{2}h \sum_{k=1}^{N}[f''(x_{k-1}) + f''(x_k)] + O(h^2)$$

$$\frac{1}{6}h^2 \int_a^b f''(x)dx = \frac{1}{12}h^3 \sum_{k=1}^{N}[f''(x_{k-1}) + f''(x_k)] + O(h^4)$$

$$\frac{1}{12}h^3 \sum_{\mathrm{k}=1}^{\mathrm{N}}[f''(x_{k-1}) + f''(x_k)] = \frac{1}{6}h^2[f'(b) - f'(a)] + O(h^4)$$

By substitution, we have

$$\text{error} = \frac{1}{12}h^2[f'(a) - f'(b)] + O(h^4)$$

The approximation error is $\epsilon = \frac{1}{12}h^2[f'(a) - f'(b)]$.

Supplementary

Euler–Maclaurin formula

$f(x)$ is $2N$ times continuously differentiable on $[a, b]$

$$\int_a^b f(x)\mathrm{d}x = h\left(\frac{1}{2}f(a) + \sum_{j=1}^{n-1} f(x_j) + \frac{1}{2}f(b)\right) + \sum_{k=1}^{N-1} \frac{B_{2k}}{(2k)!}\left[f^{(2k-1)}(a) - f^{(2k-1)}(b)\right] h^{2k} + O(h^{2N})$$

$B_k' s$ are the Bernoulli numbers

The trapezoidal rule introduces the error of order $O(h^2)$

Let I be the true value of the integral.

If $N_2 = 2N_1$

For step size $\mathrm{h}_1 = \frac{\mathrm{b-a}}{\mathrm{N}_1}$
We got $\mathrm{I} \simeq \mathrm{I}_1 \quad \mathrm{I} = \mathrm{I}_1 + \mathrm{c}\mathrm{h}_1^2$

For step size $\mathrm{h}_2 = \frac{\mathrm{b-a}}{\mathrm{N}_2} = \frac{1}{2}\mathrm{h}_1$
We got $\mathrm{I} \simeq \mathrm{I}_2 \quad \mathrm{I} = \mathrm{I}_2 + \mathrm{c}\mathrm{h}_2^2$

Then we have $I_2 - I_1 = ch_1^2 - ch_2^2 = 3ch_2^2$

$$\epsilon_2 = ch_2^2 = \frac{1}{3}(I_2 - I_1)$$

The Simpson's rule has error of order $O(h^4)$ (will be shown later)

Let I be the true value of the integral.

If $N_2 = 2N_1$

For step size $\mathrm{h}_1 = \frac{\mathrm{b-a}}{\mathrm{N}_1}$
We got $\mathrm{I} \simeq \mathrm{I}_1 \quad \mathrm{I} = \mathrm{I}_1 + \mathrm{ch}_1^4$

For step size $\mathrm{h}_2 = \frac{\mathrm{b-a}}{\mathrm{N}_2} = \frac{1}{2}\mathrm{h}_1$
We got $\mathrm{I} \simeq \mathrm{I}_2 \quad \mathrm{I} = \mathrm{I}_2 + \mathrm{ch}_2^4$

Then we have $I_2 - I_1 = ch_1^4 - ch_2^4 = 15ch_2^4$

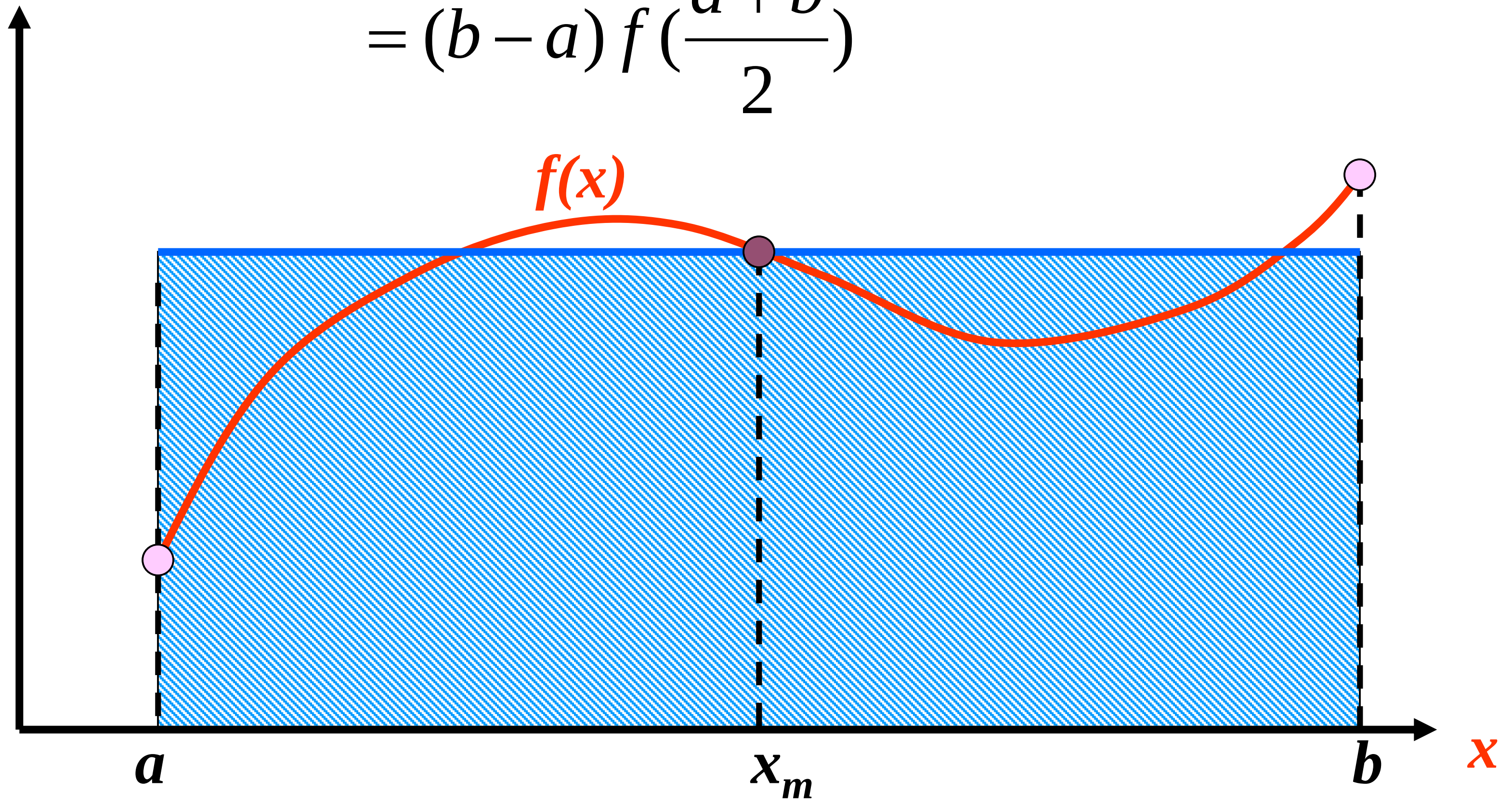
$$\epsilon_2 = ch_2^4 = \frac{1}{15}(I_2 - I_1)$$

Midpoint Rule

Newton-Cotes Open Formula

$$\int_a^b f(x)dx \approx (b-a)f(x_m)$$

$$= (b-a)f(\frac{a+b}{2})$$



Composite Mid-point Rule

$$\int_{x_1}^{x_N} f(x)dx = h\left[f_{3/2} + f_{5/2} + f_{7/2} + \cdots + f_{N-3/2} + f_{N-1/2} \right] + O\left(h^2\right)$$

The error series is, again, entirely even in *h*

Second Euler-Maclaurin summation formula:

$$\int_{x_1}^{x_N} f\left(x\right)dx = h\left[f_{3/2} + f_{5/2} + f_{7/2} + \cdots + f_{N-3/2} + f_{N-1/2} \right]$$
$$+ \frac{B_2 h^2}{4}\left(f'_N - f'_1\right) + \cdots + \frac{B_{2k} h^{2k}}{\left(2k\right)!}\left(1 - 2^{-2k+1}\right)\left(f_N^{(2k-1)} - f_1^{(2k-1)}\right) + \cdots$$

Choosing the number of steps

1. We want to get the most accurate calculation in the given amount of time.

2. We want to calculate the value of an integral of a given accuracy. We need to avoid using more steps than are necessary.

In general, we start off by evaluating the integral with some small number of steps N_1. Then we double the number to $\mathrm{N}_2 = 2N_1$. The approximate error is $(I_2 - I_1)/3$. If the error is small enough to satisfy our accuracy requirements, then we're done. If not, we keep on doubling until we achieve the required accuracy. The error on the *i*th step of the process is

$$\epsilon_i = \frac{1}{3}(I_i - I_{i-1})$$

The method is good because we no need to recalculate the entire integral again. We can reuse our previous calculation.

For trapezoidal rule,

$$
\begin{aligned}
I_i &= h_i\left[\frac{1}{2}f(a)+\frac{1}{2}f(b)+\sum_{k=1}^{N_i-1} f(a+kh_i)\right] \\
&= h_i\left[\frac{1}{2}f(a)+\frac{1}{2}f(b)+\sum_{\substack{k\text{ even}\\ 2\ldots N_i-2}} f(a+kh_i)+\sum_{\substack{k\text{ odd}\\ 1\ldots N_i-1}} f(a+kh_i)\right] \\
&= \frac{1}{2}h_{i-1}\left[\frac{1}{2}f(a)+\frac{1}{2}f(b)+\sum_{k=1}^{N_{i-1}-1} f(a+kh_{i-1})\right]+h_i\sum_{\substack{k\text{ odd}\\ 1\ldots N_i-1}} f(a+kh_i)
\end{aligned}
$$

$$
\therefore I_i = \frac{1}{2}I_{i-1}+h_i\sum_{\substack{k\text{ odd}\\ 1\ldots N_i-1}} f(a+kh_i)
$$

Similarly for Simpson's rule, we define

$$S_i = \frac{1}{3}\left[f(a) + f(b) + 2 \sum_{\substack{k \text{ even} \\ 2 \ldots N_i - 2}} f(a + kh_i)\right]$$

$$T_i = \frac{2}{3} \sum_{\substack{k \text{ odd} \\ 1 \ldots N_i - 1}} f(a + kh_i)$$

$$S_i = S_{i-1} + T_{i-1}$$

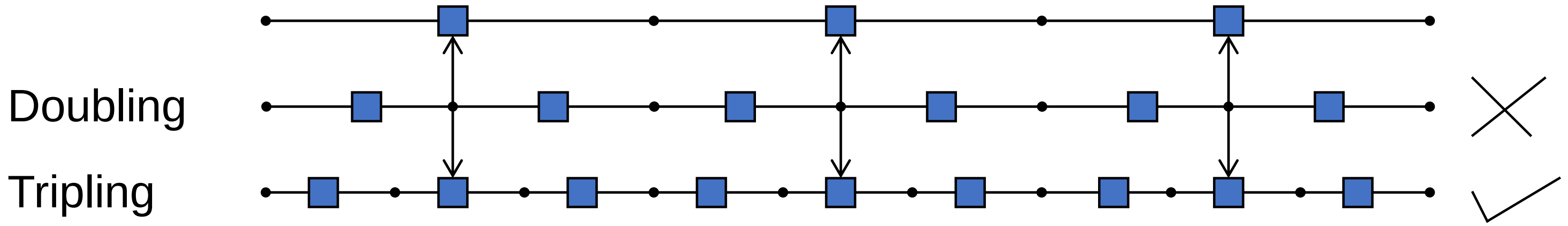
$$I_i = h_i(S_i + 2T_i)$$

Remark

- For composite mid-point rule, need tripling instead of doubling:

$$\int_{x_1}^{x_N} f(x)dx = h\left[f_{3/2} + f_{5/2} + f_{7/2} + \cdots + f_{N-3/2} + f_{N-1/2} \right] + O\left(h^2\right)$$

Doubling the number of steps cannot have the benefit of previous evaluations
Have to triple the number of steps



Higher-order integration methods

As we have seen, the trapezoidal rule is based on approximating an integrand $f(x)$ with straight line segments, while Simpson's rule uses quadratics. We can create higher-order rule by using higher-order polynomials. In general, using an N-point rule allows us to approximate the integrand by a unique polynomial of degree $N - 1$.

$$\int_a^b f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$

x_k are the positions of the sample points at which we calculate the integrand and the w_k are some set of weights.

Degree	Polynomial	Coefficients
1 (trapezoidal rule)	Straight line	1/2,1,1,…,1,1/2
2(Simpson's rule)	Quadratic	1/3,4/3,2/3,4/3,…,4/3,1/3
3	Cubic	3/8,9/8,9/8,3/4,…,9/8,3/8
4	Quartic	14/45,64/45,8/15,64/45,28/45,…,64/45,14/45

Romberg integration

For trapezoidal rule, c is a constant

$$ch_i^2 = \frac{1}{3}(I_i - I_{i-1})$$
$$I = I_i + ch_i^2 + O(h_i^4)$$

We are including the $O(h_i^4)$term to remind us of the next term in the series. (Remember that there are only even-order terms in this series.)

$$I = I_i + \frac{1}{3}(I_i - I_{i-1}) + O(h_i^4)$$

Let us define our notation,

$$R_{i,1} = I_i$$
$$R_{i,2} = I_i + \frac{1}{3}(I_i - I_{i-1}) = R_{i,1} + \frac{1}{3}\left(R_{i,1} - R_{i-1,1}\right)$$

Thus

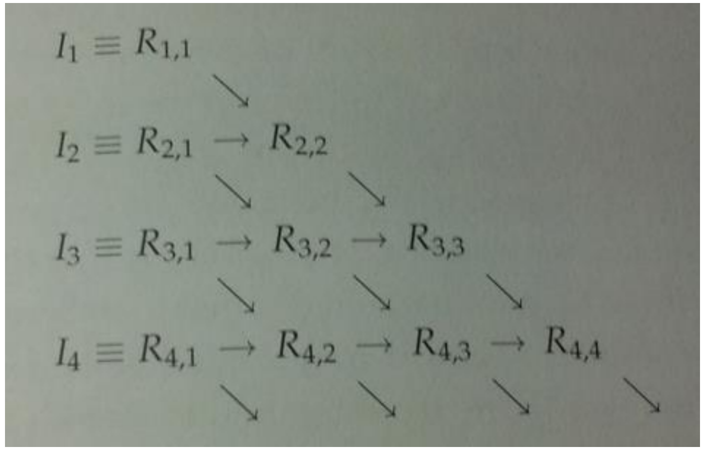
$$I = R_{i,2} + c_2 h_i^4 + O(h_i^6)$$

By repeating the process, we get the general form

$$I = R_{i,m+1} + O(h_i^{2m+2})$$

$$R_{i,m+1} = R_{i,m} + \frac{1}{4^m - 1}\left(R_{i,m} - R_{i-1,m}\right)$$

The diagram below shows which values $R_{i,m}$ are needed to calculate further *R*s:



- The payoff is a value for the integral that is accurate to much higher order in *h* that the simple trapezoidal rule. It can significantly reduce the time needed to evaluate integral because it reduces the number of trapezoidal rule steps we have to do.
- Its limitation is that it gives no advantage for the integral *f*(*x*) which is poorly behaved, containing wild fluctuations, for instance, or singularities, or if it is noisy. This method works best in case the series expansion of the integral converge rapidly.

Remark

$$
\begin{aligned}
I_i + \frac{1}{3}(I_i - I_{i-1}) &= \frac{4}{3}I_i - \frac{1}{3}I_{i-1} \\
&= \frac{4}{3}h_i\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N_i-1} f(a+kh_i)\right] - \frac{1}{3}h_{i-1}\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N_{i-1}-1} f(a+kh_{i-1})\right] \\
&= \frac{4}{3}h_i\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N_i-1} f(a+kh_i)\right] - \frac{2}{3}h_i\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{\frac{N_i}{2}-1} f(a+2kh_i)\right] \\
&= \frac{4}{3}h_i\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N_i-1} f(a+kh_i)\right] - \frac{2}{3}h_i\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{\text{even } k=2}^{N_i-2} f(a+kh_i)\right] \\
&= \frac{1}{3}h_i\left[2f(a) + 2f(b) + \sum_{k=1}^{N_i-1} 4f(a+kh_i)\right] + \frac{1}{3}h_i\left[-f(a) - f(b) - \sum_{\text{even } k=2}^{N_i-2} 2f(a+kh_i)\right] \\
&= \frac{1}{3}h_i\left[f(a) + f(b) + \sum_{\text{odd } k=1}^{N_i-1} 4f(a+kh_i) + \sum_{\text{even } k=2}^{N_i-2} 2f(a+kh_i)\right]
\end{aligned}
$$

is just the Simpson's rule

Hence error of Simpson's rule is $O(h^4)$

Non-uniform sample points

Suppose we are given a non-uniform set of N points and we wish to create an integration rule. We can use the method of interpolating polynomials.

$$\phi_k = \prod_{\substack{m=1\ldots N \\ m\neq k}} \frac{x - x_m}{x_k - x_m}$$

$$= \frac{x - x_1}{x_k - x_1} \times \cdots \times \frac{x - x_{k-1}}{x_k - x_{k-1}} \times \frac{x - x_{k+1}}{x_k - x_{k+1}} \times \cdots \times \frac{x - x_N}{x_k - x_N}$$

$$\phi_k(x_m) = \begin{cases} 1 & if \;\; m=k \\ 0 & if \;\; m\neq k \end{cases} = \delta_{km}$$

$$\Phi(x) = \sum_{k=1}^{N} f(x_k)\phi_k(x)$$

Thus

$$\Phi(x_m) = \sum_{k=1}^{N} f(x_k)\phi_k(x_m) = \sum_{k=1}^{N} f(x_k)\delta_{km} = f(x_m)$$

In other words $\Phi(x)$ is the unique polynomial of degree $N-1$ that fits the integrand $f(x)$ at all of the sample points (N points).

The weights can be deduced by

$$\int_a^b f(x)dx \approx \int_a^b \Phi(x)dx = \int_a^b \sum_{k=1}^{N} f(x_k)\phi_k(x)dx = \sum_{k=1}^{N} f(x_k) \int_a^b \phi_k(x)dx$$

$$w_k = \int_a^b \phi_k dx$$

There is no general closed-form formula for the integrals of the interpolating polynomials. We may have to perform them on the computer, using one of our other integration methods, such as Simpson's rule or Romberg integration. The important point to notice is that WE ONLY HAVE TO CALCULATE THE WEIGTHS w_k ONCE, and then we can use them to integrate as many different functions over the given integration domain as we like.

For historical reason, typically one gives samples and weights arranged in a standard interval,

$$t = -1 \text{ to } t = +1, \qquad -1 \le t_k \le 1, \qquad w_k = \int_{-1}^{1} \phi_k(t)dt$$

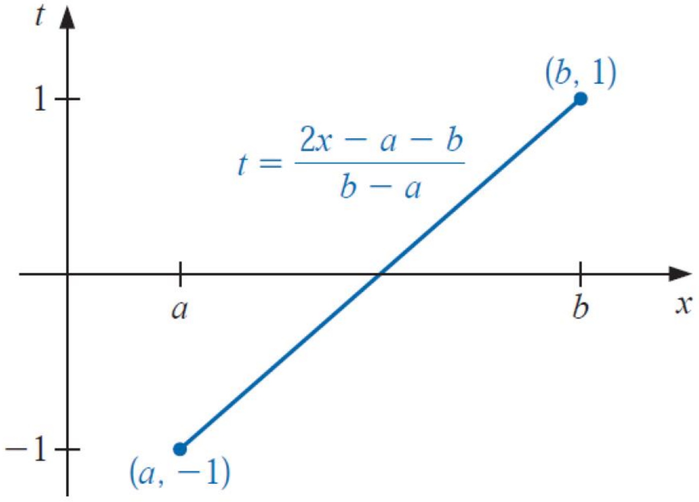
For a general domain $x = a \ to \ x = b$, define

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

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

$$\approx \frac{b-a}{2}\sum_{k=1}^{N} w_k f\big(x(t_k)\big)$$

$$= \sum_{k=1}^{N} w_k' f\big(x(t_k)\big)$$

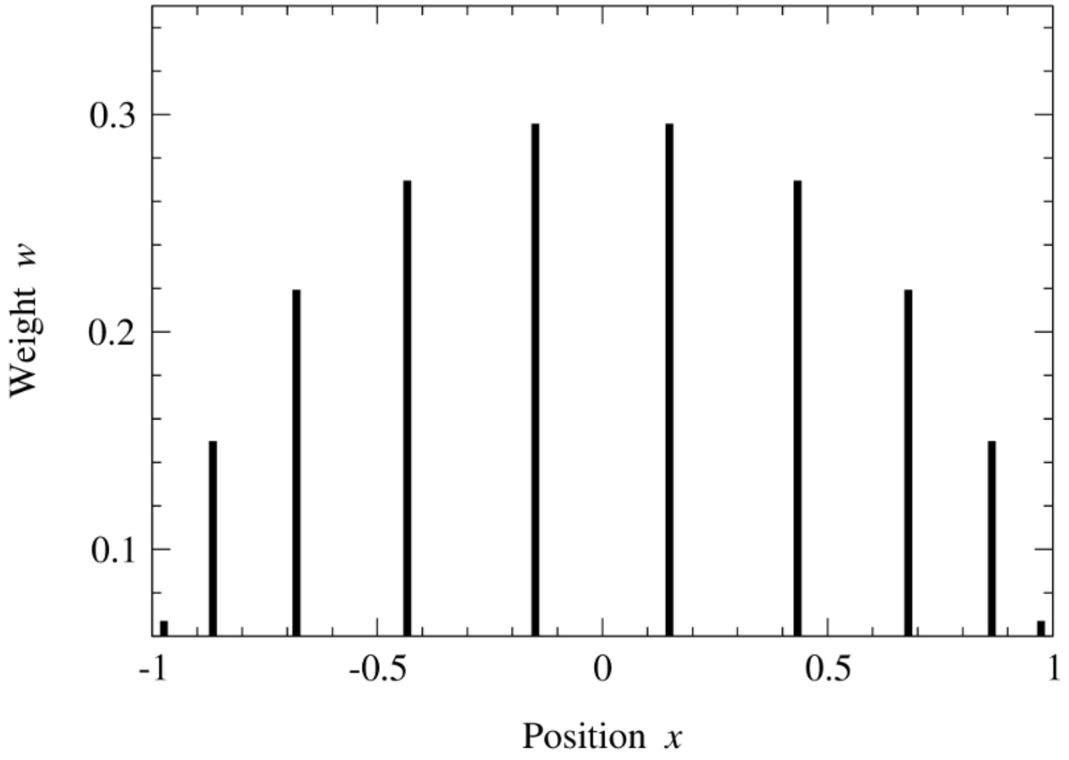


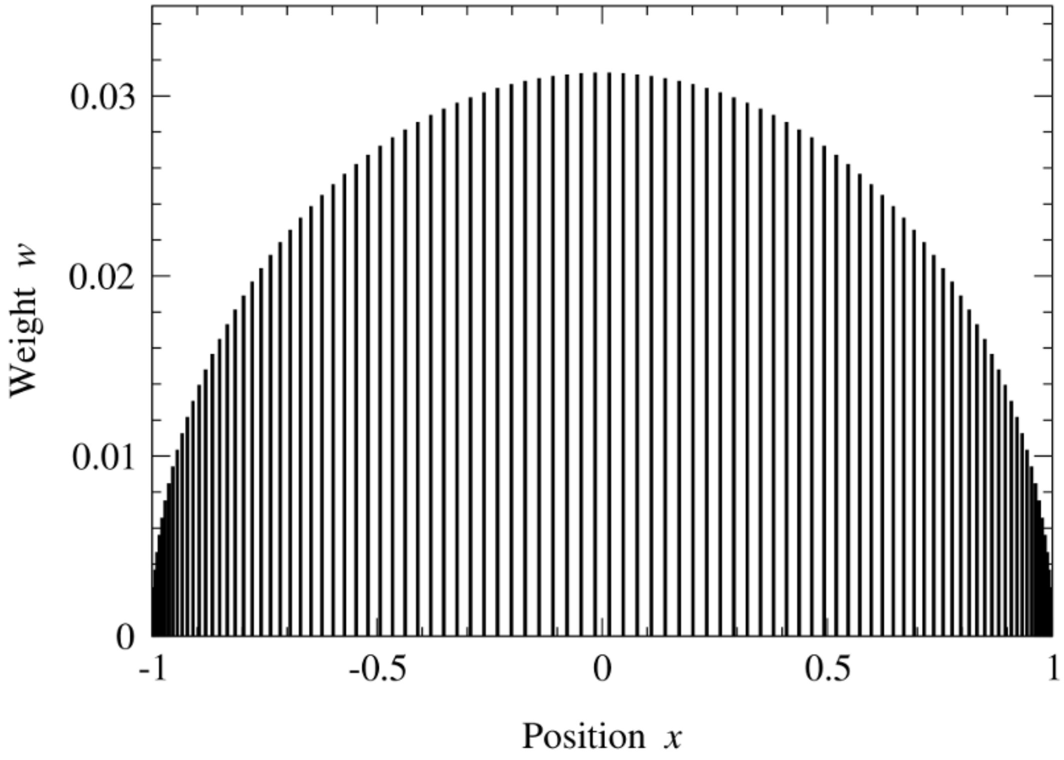
where

$$w_k' = \frac{1}{2}(b-a)w_k$$

Sample points for Gaussian Quadrature

We still have N degrees of freedom of choosing the positions of the sample points. It can be shown that they can be chosen so that our integration rule is exact for all polynomial integrands up to and including order $2N - 1$.





An Example

interval of integration is $[-1, 1]$ $\qquad n = 2$

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

we need c_1, c_2, x_1, and x_2, so that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\,dx = 2, \qquad c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\,dx = 0,$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}, \quad \text{and} \quad c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3\,dx = 0.$$

Solving the system: $\quad c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad$ and $\quad x_2 = \frac{\sqrt{3}}{3}$

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

Legendre Polynomials

a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots,\}$ with properties:

(1) For each n, $P_n(x)$ is a monic polynomial of degree n.

(2) $\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

The first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - \frac{1}{3},$$

$$P_3(x) = x^3 - \frac{3}{5}x, \quad \text{and} \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

Theorem

- The N zeros $x_1, x_2, \dots x_N$ of the N-th Legendre Polynomial $P_N(x)$ all lie in the interval $(-1,1)$
- If $P(x)$ is any polynomial of degree less than $2N$, then

$$\int_{-1}^{1} P(x)dx = \sum_{k=1}^{N} w_k P(x_k)$$

Gaussian Quadrature:

Choose x_k to coincide with the zeros of the Nth Legendre polynomial $P_N(x)$

The corresponding weights are

$$w_k = \left[\frac{2}{1-x^2}\left(\frac{dP_N}{dx}\right)^{-2}\right]_{x=x_k}$$

Tables containing values of x_k and w_k up to about $N = 20$ can be found in books or on-line.

You can also use gaussxw.py which can be downloaded from

http://www-personal.umich.edu/~mejn/cp/programs.html

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

For example, we need to calculate $\int_0^2 (x^4 - 2x + 1)dx$. We perform the calculation with $N = 3$ sample points:

```
from gaussxw import gaussxw
def f(x):
    return x**4 - 2*x + 1

N = 3
a = 0.0
b = 2.0

# Calculate the sample points and weights, then map them to the required integration domain
x,w = gaussxw(N)
xp = 0.5*(b-a)*x + 0.5*(b+a)
wp = 0.5*(b-a)*w

# Perform the integration
s = 0.0
for k in range(N):
    s += wp[k]*f(xp[k])

print(s)
```

The strength of Gaussian Quadrature is that it gives remarkably accurate answer, even with small numbers of sample points. The disadvantage of this method is that we cannot reuse the calculations for old sample points as we did with trapezoidal rule, since the sample points are not uniformly distributed.

Errors on Gaussian Quadrature

The approximation error improves by a factor of c/N^2 when we increase the number of samples by just one, where c is a constant depends on the shape of integrand and size of the domain of integration. This means we converge extremely quickly on the true value of the integral.

However, the function being integrated must be reasonably smooth. Since Gaussian quadrature looks only at the values of the function at the sample points, for rapidly varying functions one needs to use enough sample points to capture the variation.

Example

Consider the integral $\int_1^3 x^6 - x^2 \sin(2x)\, dx$

Changing variables from $x \in [1,3]$ to $t \in [-1,1]$: $\quad x = t + 2$

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx = \int_{-1}^1 (t+2)^6 - (t+2)^2 \sin(2(t+2))\, dt.$$

Gaussian quadrature with $n = 2$

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx \approx f(-0.5773502692+2) + f(0.5773502692+2) = 306.8199344$$

Gaussian quadrature with $n = 3$,

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx \approx 0.\overline{5} f(-0.7745966692+2) + 0.\overline{8} f(2) + 0.\overline{5} f(0.7745966692+2)$$

$$= 317.2641516$$

The exact value of the integral is $\int_1^3 x^6 - x^2 \sin(2x)\, dx = 317.3442466\cdots$

Newton-Cotes formula with $n = 1$ (two points)

$$\frac{2}{2}\left[f(1) + f(3)\right] = 731.6054420$$

Newton-Cotes formula with $n = 2$ (three points)

$$\frac{2}{6} * \left[f(1) + 4f(2) + f(3)\right] = 333.2380940$$

Remark: Choosing an integration method

The trapezoidal rule:

It is trivial to program and hence is a good choice when you need a quick answer for an integral. It is not very accurate. It is good choice for poorly behaved functions-those that vary widely, contain singularities, or are noisy.

Simpson's rule:

It gives greater accuracy than the trapezoidal rule with the same number of sample points. It can lead to problems when the integrand is noisy or not smooth.

Romberg integration:

It gives exceptionally accurate estimates of integrals with a minimum number of sample points, plus error estimates that allow you to halt the calculation once you have achieved a desired accuracy. It will not work for wildly varying integrands, noisy integrands, singularities…

Gaussian quadrature:

It has many advantages as Romberg integration as well as the same disadvantages. The integration points are unequally spaced. Its hard work lies in the calculation of the integration points and weights.

Integral over infinite range

Use the method of change of variables.

1. $\int_a^\infty f(x)dx$

Let $x = \frac{z}{1-z} + a$, $z = \frac{x-a}{x-a+1}$

$$\int_a^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f\left(\frac{z}{1-z} + a\right) dz$$

2. $\int_{-\infty}^a f(x)dx$

Let $x = \frac{z}{1+z} + a$, $z = -\frac{x-a}{x-a-1}$

$$\int_{-\infty}^a f(x)dx = \int_{-1}^0 \frac{1}{(1+z)^2} f\left(\frac{z}{1+z} + a\right) dz$$

3. $\int_{-\infty}^{\infty} f(x)dx$

Method 1: Split it into two integrals by cutting at some point and then apply (1) and (2).

Method 2: Let $x = \frac{z}{1-z^2}$,

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-1}^{1} \frac{1+z^2}{(1-z^2)^2} f\left(\frac{z}{1-z^2}\right) dz$$

Method 3: Let $x = \tan z$

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-\pi/2}^{\pi/2} \frac{f(\tan z)}{\cos^2 z} dz$$

Example: To integrate

$$I = \int_0^\infty e^{-x^2} dx$$

Let $x = \frac{z}{1-z}$, $z = \frac{x}{x+1}$,

$$I = \int_0^1 \frac{e^{-z^2/(1-z)^2}}{(1-z)^2} dz$$

Use Gaussian Quadrature:

```
from gaussxw import gaussxwab

from math import exp

def f(z):

    return exp(-z**2/(1-z)**2)/(1-z)**2

N = 50

a = 0.0

b = 1.0

x,w = gaussxwab(N,a,b)

s = 0.0

for k in range(N):

    s += w[k]*f(x[k])

print(s)
```

Multiple Integrals

Consider for example the integral

$$I = \int_0^1 \int_0^1 f(x,y)dx\,dy$$

We can define

$$F(y) = \int_0^1 f(x,y)dx$$

$$I = \int_0^1 F(y)dy$$

If we do the integral by Gaussian quadrature with the same number N of points for both x and y integrals, we have

$$F(y) \approx \sum_{i=1}^{N} w_i f(x_i, y) \quad \text{and} \quad I \approx \sum_{j=1}^{N} w_j F(y_j)$$

We get the Gauss-Legendre product formula

$$I \approx \sum_{i=1}^{N} \sum_{j=1}^{N} w_i w_j f(x_i, y_j)$$

The figure shows the sample points for Gaussian quadrature in two dimensions. If one applies the Gauss-Legendre product formula to integrate the function $f(x, y)$ in two dimensions, using $N = 10$ points along each axis.