Numerical integration

Finding a derivative analytically is simple, integration difficult.

The situation is exactly opposite when using numeical methods.

Integration is addition, which is a smoothing operation: random errors of data tend to cancel out.

Differentiation requires difference of nearly equal quantitites, which will enhance errors. Cf. image processing where sharpening an image will increase noise.

When dealing with observational data, it may have to be smoothened with a proper filter or replaced by a function to be fitted to the data. In differentiation this is necesary, but usually not in integration.

A function f is integrable in the interval $[x_1 = a, x_n = b]$, if the Riemann sum

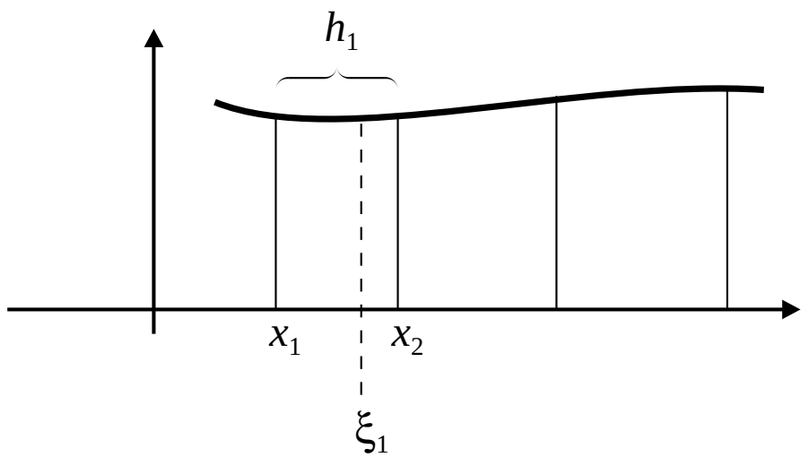
$$R = \sum_{i=1}^{n-1} f(\xi_i) h_i,$$

where

$$h_i = x_{i+1} - x_i, \quad \xi_i \in [x_i, x_{i+1}],$$

has a limit when $h = \max_i\{h_i\} \to 0$.

Different methods for integration are obtained by choosing the subdivisions and the points ξ_i in different ways.



Divide the interval into equal slices of width h.

1) Evaluate the integrand at the beginning of each subdivision:

$$\int_{x_0}^{x_n} f(x)\,dx = h(f(x_0) + f(x_0 + h) + \ldots + f(x_0 + (n-1)h)).$$

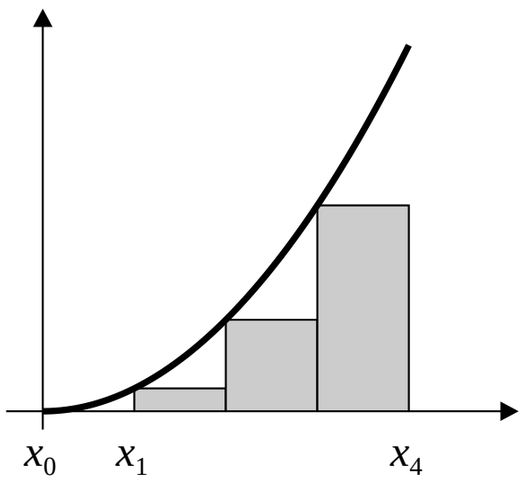
Example:

$$I = \int_0^1 x^2\,dx.$$

The exact value is 1/3. Find the integral by dividing the interval into four parts.

$$I_4 = \frac{1}{4}\left(0 + \frac{1}{16} + \frac{1}{4} + \frac{9}{16}\right) = \frac{14}{64} \approx 0.219.$$

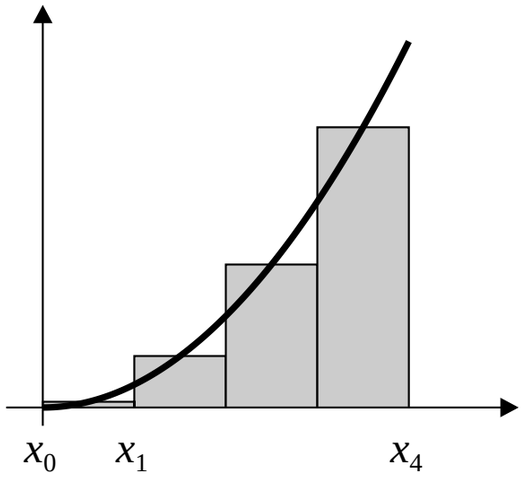
Since the integrand is an increasing function in the whole interval, evaluating it at the bginning of each subinterval gives a value that is too small.



2) Evaluate the integrand at the midpoint:

$$\int_{x_0}^{x_n} f(x)\,dx = h(f(x_0 + h/2) + f(x_0 + 3h/2) + \ldots).$$

$$I_4 = \frac{1}{4}\left(\frac{1}{64} + \frac{9}{64} + \frac{25}{64} + \frac{49}{64}\right) = \frac{21}{64} \approx 0.328.$$



The trapezoidal tule

Replace the integrand by an interpolation polynomial

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_n} P_k(x)\,dx.$$

When $k = 1$, the integral over one subdivision is

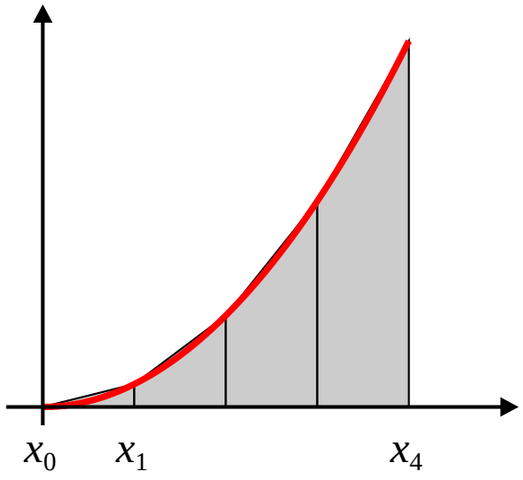
$$\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} (f_0 + s\Delta f_0)\,dx$$

When we make the substitution $x = hs$, $dx = h\,ds$ the integral becomes

$$\begin{aligned}\int_{x_0}^{x_n} f(x)\,dx &= h\int_{s=0}^{s=1} (f_0 + s\Delta f_0)\,ds \\ &= h(f_0 + \frac{1}{2}\Delta f_0)\,ds \\ &= \frac{h}{2}(2f_0 + (f_1 - f_0)) = \frac{h}{2}(f_0 + f_1).\end{aligned}$$

The integral over the whole interval is

$$\begin{aligned}\int f(x)\,dx &= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{n-1} + f_n) \\ &= \frac{h}{2}(f(x_0) + 2f(x_0+h) + 2f(x_0+2h) + \ldots \\ &\quad + 2f(x_0+(n-1)h) + f(x_0+nh)).\end{aligned}$$



Error estimate

The error of the interpolation polynomial is at most of the order of the first omitted term.

$$\Delta f_0 = f_1 - f_0 \approx h\frac{df}{dx}$$
$$\Delta^2 f_0 = \Delta f_1 - \Delta f_0 \approx h^2\frac{d^2 f}{dx^2}$$
$$\vdots$$
$$\Delta^n f_0 \approx h^n\frac{d^n f}{dx^n}$$

The third term of the Newton-Gregory interpolation polynomial is

$$\frac{s(s-1)}{2}\Delta^2 f_0 = \frac{s(s-1)}{2}h^2 f''(\xi),$$

where $x_0 \leq \xi \leq x_s$.

Integrate this over one subinterval to get the *local error*:

$$\begin{aligned}
&\int_{x_0}^{x_1} \frac{s(s-1)}{2} h^2 f''(\xi)\, dx \\
&= h^2 f''(\xi) h \int_0^1 \frac{s^2 - s}{2}\, ds \\
&= -\frac{1}{12} h^3 f''(\xi).
\end{aligned}$$

There are $1/h$ subintervals; thus the *global erros* is of the order $h^2 f''(\xi)$.

In the example the integral is

$$I_4 = \frac{1}{8}\left(\frac{1}{16} + \frac{1}{2} + \frac{9}{8} + 1\right) = \frac{43}{6 \times 16} \approx 0.336.$$

The second derivative of the function is identically 2. Thus the global error is at most

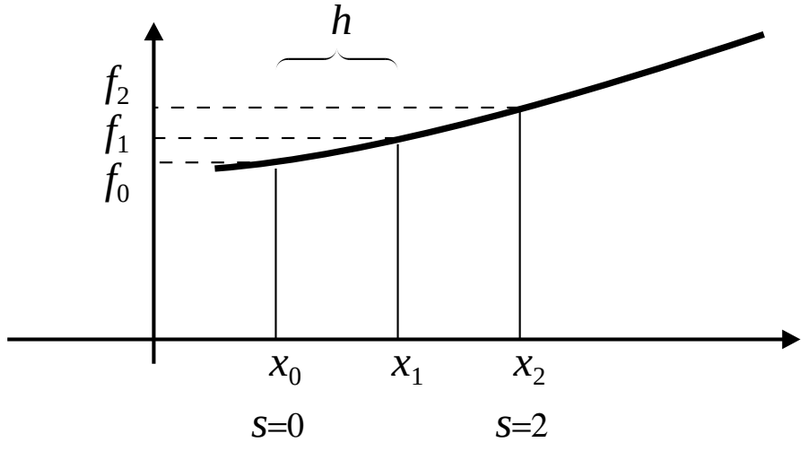
$$\frac{1}{12} h^2 f''(\xi) = \frac{1}{12}\frac{1}{4^2} 2 = 0.010.$$

Simpson's rule

If we use more complex curves they can represent the integrand more closely. An obvious improvement is a quadratic polynomial.

First find the integral over two subintervals. According to a former interpolation formula we have

$$f(x) \approx f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0.$$



$$\begin{aligned}
\int_{x_0}^{x_2} f(x)\,dx &\approx \int_{x_0}^{x_2} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 \right) dx \\
&= h \int_0^2 \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 \right) ds \\
&= h(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0) \\
&= \frac{h}{3}(6f_0 + 6\Delta f_0 + \Delta^2 f_0)
\end{aligned}$$

Make the substitutions

$$\begin{aligned}
\Delta f_0 &= f_1 - f_0 \\
\Delta^2 f_0 &= \Delta f_1 - \Delta f_0 = (f_2 - f_1) - (f_1 - f_0) \\
&= f_0 - 2f_1 + f_2.
\end{aligned}$$

The integral over two subdivisions is

$$\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2)).$$

The integral over the whole interval is

$$\begin{aligned}&\int_{x_0}^{x_n} f(x)\,dx\\ &\approx \frac{h}{3}\big(f(x_0)+4f(x_0+h)+2f(x_0+2h)+4f(x_0+3h)+2f(x_0+4h)+\ldots\\ &\qquad 4f(x_0+(n-1)h)+f(x_0+nh)\big).\end{aligned}$$

The number of subintervals must be even.

The global error is of the order $O(h^4)$.

Example:

$$I_4=\frac{1}{12}\left(4\times\frac{1}{16}+2\times\frac{1}{4}+4\times\frac{9}{16}+1\right)=\frac{16}{12\times 4}=\frac{1}{3}.$$

```
program simpson
  implicit none
  integer i
  do i=4,10
    write(*,*) i, simpsonint(0.0, 1.0, i)
  end do
contains

real function f(x)
  ! integrand
  real, intent(in) :: x
  f=x**4
end function
```

```
real function simpsonint(a, b, n)
 ! integrate f(x) over [a, b] using Simpson's rule
 ! with n subintervals (n must be even)
 real, intent(in) :: a, b
 integer, intent(in) :: n

 real :: h, &   ! step length
      s2, s4  ! partial sums
 integer i

 if (2*(n/2) /= n) then
   write(*,*) 'number of subdivisions must be even:',n
   simpsonint=0.0
   return
end if

h = (b-a)/n
s2=0.0
s4=0.0
do i=1,n-1,2
  s4=s4+f(a+i*h)
end do
```

```
  do i=2,n-2,2
    s2=s2+f(a+i*h)
  end do
  simpsonint = (h/3)*(f(a)+f(b)+2*s2+4*s4)
end function
end program
```

```
 4 0.200520843
 number of subdivisions must be even: 5
 5 0.00000000E+00
 6 0.200102881
 number of subdivisions must be even: 7
 7 0.00000000E+00
 8 0.200032562
 number of subdivisions must be even: 9
 9 0.00000000E+00
 10 0.200013325
```

Romberg integration

Find the integral with some simple method using two different step lengths. These values are then used to extrapolate a more accurate value.

Let I be the exact value of the integral. It can be shown that in the trapezoidal method the value as a function of the step size $R_0(h)$ is

$$R_0(h) = I + C_2 h^2 + C_4 h^4 + \ldots,$$

where the coefficients C_i are independent of h.

$$R_0(h/2) = I + C_2 \frac{h^2}{4} + C_4 \frac{h^4}{16} + \ldots,$$

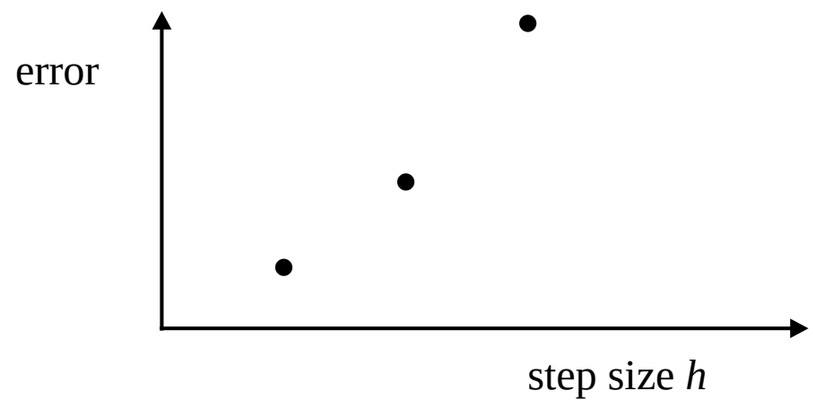
Use these to calculate a linear combination

$$\begin{aligned} R_1(h) &= \frac{1}{3}\left(4R_0(h/2) - R_0(h)\right) \\ &= I + C_4' h^4 + \ldots, \end{aligned}$$

The initial method is of the order h^2, but their combination of the order h^4.

If the data consists of values tabulated at intervals of h, compute the integral using steps $2h$ and h.

The method can be generalized to higher orders.



Newton–Cotes methods

All previous methods can be expressed in the forma

$$I = \sum w_i f(x_i),$$

where $(x_i), i = 0, \ldots, n$ is some suitably selected set of points.

If the points x_i are equally spaced we get integration methods known as the Newton–Cotes methods.

All the previous methods belong to this group. They are simple and easy to program. For many purposes they are perfectly useful. The disadvantage is that high precision requires a short step size, which makes the programs relatively slow.

Gaussian quadrature

Accuracy can be improved by choosing the points x_i in a more general way.

Assume that the function is a polynomial whose degree is at most n. We'll try to find such points x_i and coefficients w_i, that $\sum w_i f(x_i)$ will give exactly correct values for the integrals of the polynomial.

Example: use two points only, and take a symmetric interval $[-1, 1]$.

If the formula is to give correct values to all polynomials up to degree n, it has to give correct values also to the integrals of 1, x, x^2, ..., x^n:

$$\int_{-1}^{1} 1\,dx = 2 = w_1 + w_2,$$
$$\int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2,$$
$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2,$$
$$\int_{-1}^{1} x^3\,dx = 0 = w_1 x_1^3 + w_2 x_2^3,$$

This has four equations and four unknowns, w_1, w_2, x_1 and x_2. The second and fourth equation are satisfied if we choose $x_2 = -x_1$ and $w_1 = w_2$. Then the first equation gives $w_1 = w_2 = 1$, and the third one $x_1 = -x_2 = 1/\sqrt{3}$.

General 3rd degree polynomials are linear combinations of the previous functions. Thus for an arbitrary 3rd degree polynomial p_3 we have

$$\int_{-1}^{1} p_3(x)\,dx = p_3\left(\frac{1}{\sqrt{3}}\right) + p_3\left(-\frac{1}{\sqrt{3}}\right).$$

Let's try:

$$\begin{aligned}
&\int_{-1}^{1} (x^3 + 2x^2 + 1)\,dx = \\
&\left|_{-1}^{1} \frac{x^4}{4} + \frac{2x^3}{3} + x = \right. \\
&= \frac{1}{4} + \frac{2}{3} + 1 - \left(\frac{1}{4} - \frac{2}{3} + 1\right) \\
&= \frac{10}{3}.
\end{aligned}$$

Gaussian two point quadrature:

$$\begin{aligned}
&\int_{-1}^{1} (x^3 + 2x^2 + 1)\, dx = \\
&= \frac{1}{3\sqrt{3}} + \frac{2}{3} + 1 + \left(\frac{-1}{3\sqrt{3}} + \frac{2}{3} + 1 \right) \\
&= \frac{10}{3}.
\end{aligned}$$

For polynomials of higher degree we get corresponding equations, but solving the equations becomes laborious. Finding the points x_i directly from such equations is not practical. Therefore, the polynomials are first expressed in terms of some orthogonal set of basis functions.

If there are n points, they are roots of the Legendre polynomial $P_n(x)$.

$$
\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= \frac{1}{2}(3x^2 - 1), \\
P_3(x) &= \frac{1}{2}(5x^3 - 3x), \\
&\vdots \\
(2n+1)P_n(x) &= (n+1)P_{n+1}(x) + nP_{n-1}(x).
\end{aligned}
$$

For example, coordinates for the three point method are the roots of the equation

$$5x^3 - 3x = 0,$$

i.e.

$$\begin{aligned} x_1 &= -\sqrt{3/5} = -0.7746, \\ x_2 &= 0, \\ x_3 &= \sqrt{3/5} = 0.7746. \end{aligned}$$

Solving these each time is not efficient. Instead, pretabulated values are usually used.

The weight w_i corresponding to the point x_i is

$$w_i = \frac{2}{(1-x_i^2)[P'(x_i)]^2}.$$

The derivatives of the polynomials are obtained using the recurrence relation

$$\begin{aligned}
P_0'(x) &= 0, \\
P_1'(x) &= 1, \\
P_2'(x) &= 3x, \\
P_3'(x) &= \frac{1}{2}(15x^2 - 3), \\
&\vdots \\
P_{n+1}'(x) &= P_{n-1}'(x) + (2n+1)P_n(x).
\end{aligned}$$

An arbitrary interval can be transformed to [-1, 1] by the substitution

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

$$dy = \frac{b-a}{2}\,dt.$$

The integral ism then

$$\int_a^b f(y)\,dy = \frac{b-a}{2}\sum w_i f(y_i),$$

where

$$y_i = \left(\frac{b-a}{2}\right)x_i + \left(\frac{b+a}{2}\right),$$

Example:

$$\int_0^{\pi/2} \sin x\,dx$$

Use the three point method to evaluate this. The transformation of the interval is

$$y_i = \frac{\pi}{4}x_i + \frac{\pi}{4}.$$

To calculate the integral we need the following quantities:

i	w_i	x_i	y_i	$w_i \sin y_i$
-1	0.5555555556	-0.7745966692	0.1770313620	0.0978378406
0	0.8888888889	0.0000000000	0.7853981634	0.6285393611
1	0.5555555556	0.7745966692	1.3937649648	0.5468726838
$\sum$				1.2732498855

The integral is $(\pi/4) \times 1.2732498855 \approx 1.000008$. The exact value is 1. Using three points only we got a value the relative error of which is less than 10^{-5}.

n	x_i	w_i
2		
	0.57735 02691 89626	1.00000 00000 00000
3		
	0.00000 00000 00000	0.88888 88888 88889
	0.77459 66692 41484	0.55555 55555 55556
4		
	0.33998 10435 84856	0.65214 51548 62546
	0.86113 63115 94053	0.34785 48451 37453
5		
	0.00000 00000 00000	0.56888 88888 88889
	0.53846 93101 05684	0.47862 86704 99366
	0.90617 98459 38664	0.23692 68850 56189
6	0.23861 91860 83197	0.46791 39345 72691
	0.66120 93864 66265	0.36076 15730 48138
	0.93246 95142 03152	0.17132 44923 79171
7		
	0.00000 00000 00000	0.41795 91836 73469
	0.40584 51513 77398	0.38183 00505 05118

	0.74153 11855 99395	0.27970 53914 89277
	0.94910 79123 42759	0.12948 49661 68868
8		
	0.18343 46424 95650	0.36268 37833 78362
	0.52553 24099 16329	0.31370 66458 77887
	0.79666 64774 13627	0.22238 10344 53375
	0.96028 98564 97536	0.10122 85362 90376
9		
	0.00000 00000 00000	0.33023 93550 01260
	0.32425 34234 03809	0.31234 70770 40003
	0.61337 14327 00590	0.26061 06964 02935
	0.83603 11073 26636	0.18064 81606 94857
	0.96816 02395 07626	0.08127 43883 61575

To increase accuracy, more points are needed. Unfortunately, previously calculated values can not be used.

In the Gauss-Kronrod method $n + 1$ new points are added to the previous n points, and the old values are reused.

Multiple integrals

Onedimensional integration can be applied separately in each dimensioon.

Example: a 2-dimensional integral:

$$\begin{aligned}
&\int_a^b \int_c^d f(x,y)\,dx\,dy \\
&= \sum w_i \left(\int_c^d f(x_i,y)\,dy \right) \\
&= \sum w_i \sum w'_j f(x_i,y_j).
\end{aligned}$$

Depending on the weights and coordinates the method here can be either Gaussian or some Newton–Cotes.

When the dimension is higher than about 5, Monte Carlo methods become more efficient.

Improper integrals

For example

$$\int_0^\infty f(x)\,dx.$$

Different possibilities:

1) Find a transform $[0, \infty] \to [a, b]$.

2) Continue integration further until the result will not change.

3) Piecewise integration. The function will usually have big values only in a finite range, where a short step should be used. In addition there is a long tail where the function becomes very small, and a long step can be used.

Monte Carlo method

The value of the integral

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

estimated by the simplest method is

$$\sum_{i=0}^{n-1} \frac{f(x_i)}{n}.$$

This is the mean value of the function in the interval [0,1]. Generally, an integral is the mean value of the function times the length of the interval.

In principle we'll get the same result, if the integral is evaluated using random points t_i distributed evenly in the interval:

$$I' = \sum_{i=0}^{n-1} \frac{f(t_i)}{n}.$$

This is a random variable; its expectation is the value of the integral: $EI' = I$, When $N \to \infty$, $I' \to I$.

If we have to find an integral

$$\int_A f\, dV$$

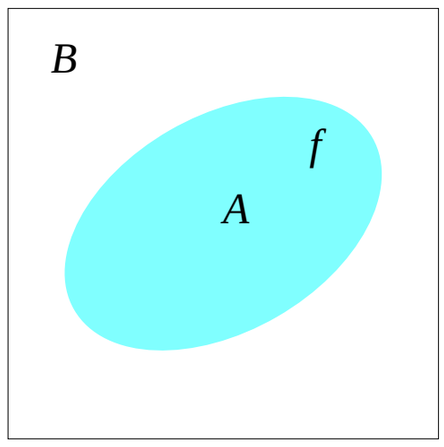
over some complicated region A, we can evaluate instead

$$\int_B g\, dV,$$

where $A \subset B$ and $g(x) = f(x)$, if $x \in A$ and 0 otherwise. An estimate of the integral is

$$I = \sum g(x_i),$$

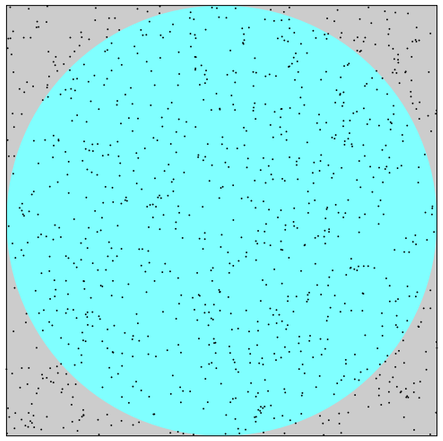
where the random numbers x_i are evenly distributed in the region B.



Example: finding the volume of an n-dimensional sphere. Generate points distributed inside a cube

$$\mathbf{r}_i = (X_1, X_2, ..., X_n).$$

Now $g(\mathbf{r}_i) = 1$, if $|\mathbf{r}_i|$ is smaller than the radius of the sphere, 0 otherwise. The sum $\sum g(\mathbf{r}_i)$ will approach the ratio of the volumes of the sphere and the surrounding cube.



nr of points	1000
inside the circle	772
πapprox	3,09

The error is proportional to $1/\sqrt{n}$. Computation can be continued as needed to obtain the required accuracy. If an ordinary method with a fixed grid is used, the whole process must be repeated if higher precision is needed.

However, the accuracy improces slowly; thus the method is not good for all problems.

The error is independent on the number of dimensions. Thus the method is useful for evaluating multidimensional integrals.

Integration of observational data

If the data is equally spaced any Newton–Cotes method can be used.

In the case of unequally spaced data methods can be modified to use variable step length. For example, the trapezoidal rule becomes

$$\int f(x)\,dx = \frac{1}{2}\Bigg((x_1 - x_0)f(x_0) + (x_2 - x_1)f(x_1) + \ldots + (x_n - x_{n-2})f(x_{n-1}) + (x_n - x_{n-1})f(x_n)\Bigg).$$

Another possibility is to fit a function to describe the data. Then any method can be applied (or the function may be analytically integrable).

If the data is a result of simulations or other heavy computations but can be evaluated at arbitrary points, it is worth considering the Gaussian quadrature.