Integrals and derivatives

While some integrals can be done analytically in closed form, most cannot. They can, however, almost always be done on a computer. Here we examine a number of different techniques for evaluating integrals and derivatives.

A) Derivatives

The basic techniques for numerical derivatives are quite simple.

Forward and backward differences

We can use the definition of a derivative to implement a numerical calculation making h very small, i.e. the forward difference:

$\frac{df}{dx} \simeq \frac{f(x+h)-f(x)}{h}$.

There is also the backward difference:

$\frac{df}{dx} \simeq \frac{f(x)-f(x-h)}{h}$.

The forward and backward differences typically give about the same answer and in many cases you can use either.

Central differences

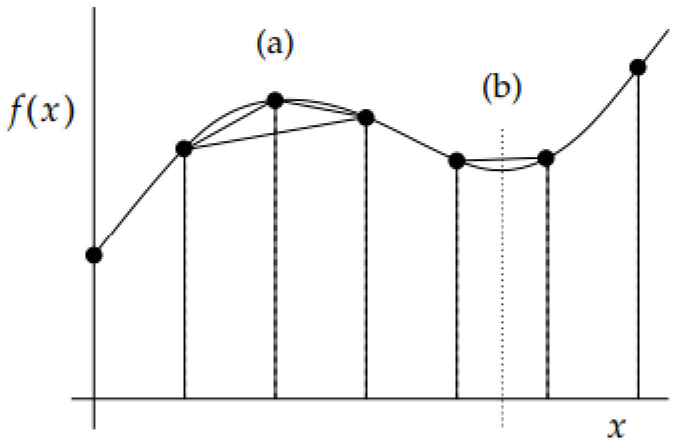
However, there is a simple improvement: the central difference.

$\frac{df}{dx} \simeq \frac{f(x+h/2)-f(x-h/2)}{h}$.

What happens if we are given a **sampled function**? If we only know the function at a set of sample points spaced a distance h apart then we must chose between calculating the forward or backward difference between adjacent samples, or the central difference between samples 2h apart:

$\frac{df}{dx} \simeq \frac{f(x+h)-f(x-h)}{2h}$.

We cannot calculate a central difference using the standard formula because we do not know the value of the function at x ± h/2. We can, however, calculate the value of the derivative at a point half way between two samples (dotted line) using the standard formula.



What happens if we would like to derive numerical approximations for the **second derivative** of a function f(x)?

Example:

Create a user-defined function f(x) that returns the value 1 + (1/2) tanh 2x, then use a central difference to calculate the derivative of the function in the range −2 ≤ x ≤ 2. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots. (Hint: In Python the tanh function is found in the math package, and it's called simply tanh.)

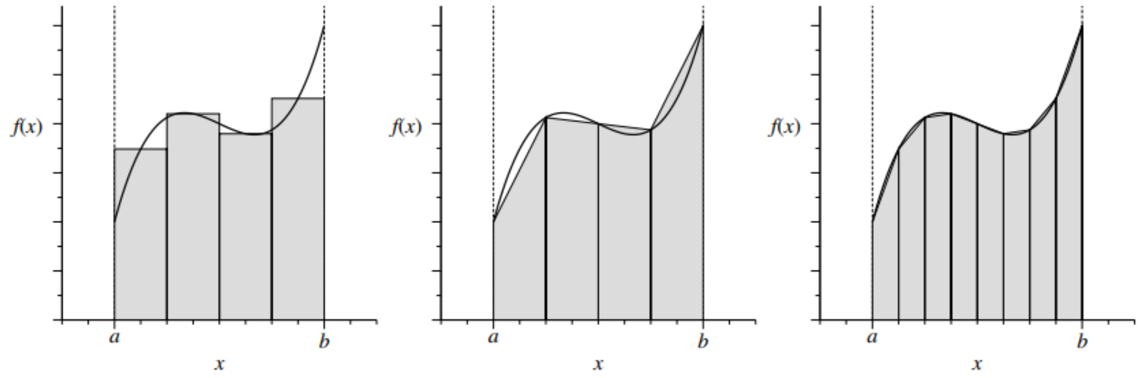
B) Integrals

The trapezoidal or trapezium rule

Suppose we have a function f(x) and we want to calculate its integral with respect to x from x = a to x = b, which we denote I(a,b):

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

This is equivalent to calculating the area under the curve of f(x) from a to b. There is no known way to calculate such an area exactly in all cases on a computer, but we can do it approximately by the method shown here:



(a) (b) (c)

We divide the area up into rectangular slices, calculate the area of each one, and then add them up. This, however, is a pretty poor approximation. The area under the rectangles is not very close to the area under the curve. A better approach, which involves very little extra work, consists of dividing the area into trapezoids rather than rectangles. The area under the trapezoids is a considerably better approximation to the area under the curve, and this approach, though simple, often gives perfectly adequate results.

Suppose we divide the interval from a to b into N slices or steps, so that each slice has width h = (b − a)/N. Then the right-hand side of the kth slice falls at a + kh, and the left-hand side falls at a + kh − h = a + (k − 1)h. Thus the area of the trapezoid for this slice is:

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

Our approximation for the area under the whole curve is the sum of the areas of the trapezoids for all N slices:

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

$$I(a,b) \simeq \frac{1}{2}h[f(a)+2f(a+h)+2f(a+2h)+\ldots+f(b)]$$

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

We can make the calculation more accurate by increasing the number of slices, though the program will also take longer to reach an answer because there are more terms in the sum to evaluate.

The trapezoidal rule is the simplest of numerical integration methods, taking only a few lines of code, and it is often perfectly adequate for calculations where no great accuracy is required. It happens frequently in physics calculations that we don't need an answer accurate to many significant figures and in such cases the ease and simplicity of the trapezoidal rule can make it the method of choice.

Example 1:

Use the trapezoidal rule to calculate the integral of $x^4 - 2x + 1$ from x = 0 to x = 2 using 10 slices or steps.

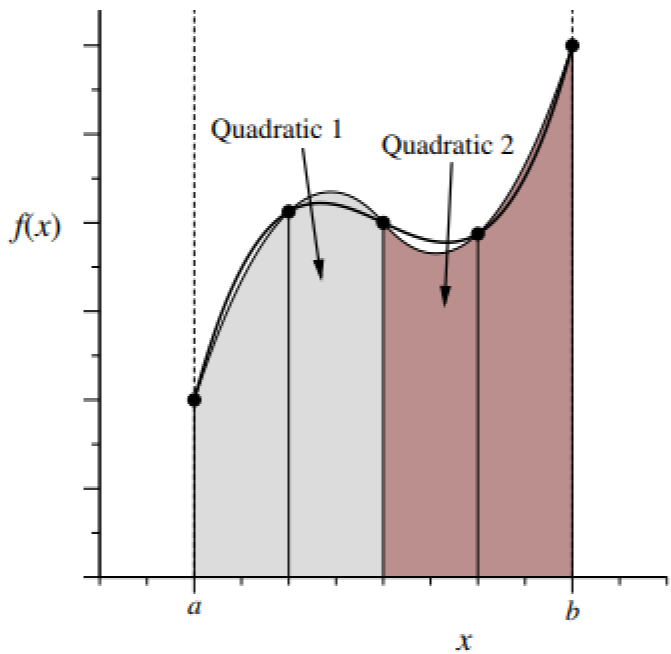
Example 2:

Download the file called **velocities.txt**, which contains two columns of numbers, the first representing time t in seconds and the second the x-velocity in meters per second of a particle, measured once every second from time t = 0 to t = 100. Write a program to use the trapezoidal rule to calculate the distance traveled by the particle in the x direction as a function of time.

The Simpson's rule

There are also cases where greater accuracy is required. We can increase the accuracy of the trapezoidal rule by increasing the number N of steps used in the calculation. But in some cases, particularly for integrands that are rapidly varying, a very large number of steps means the calculation can become slow. There are other, more advanced schemes for calculating integrals that can achieve high accuracy while still arriving at an answer quickly. One of them is the Simpson's rule.

The trapezoidal rule estimates the area under a curve by approximating the curve with straight-line segments. A better result can be achieved if we approximate the function instead with curves of some kind. Simpson’s rule does exactly this, using quadratic curves. In order to completely specify a quadratic, one needs three points. So in this method we take a pair of adjacent slices and fit a quadratic through the three points that mark the boundaries of those slices. In the following figure there are two quadratics, fitted to four slices. Simpson’s rule involves approximating the integrand with quadratics in this way, then calculating the area under those quadratics, which gives an approximation to the area under the true curve.



Suppose that our integrand is denoted f(x) and the spacing of adjacent points is h. And suppose for the purposes of argument that we have three points at x = −h, 0, and +h. If we fit a quadratic Ax**2 + B*x + C through these points, then by definition we will have:

$f(-h) = Ah^2 - Bh + C$

$f(0) = C$

$f(h) = Ah^2 + Bh + C$

Solving these equations simultaneously for A, B, and C gives

$A = \frac{1}{h^2}\left[\frac{1}{2}f(-h) - f(0) + \frac{1}{2}f(h)\right]$

$B = \frac{1}{2h}[f(h) - f(-h)]$

$C = f(0)$

and the area under the curve of f(x) from −h to +h is given approximately by the area under the quadratic:

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

Note that the final formula for the area involves only h and the value of the function at evenly spaced points, just as with the trapezoidal rule. So to use Simpson’s rule we don’t actually have to worry about the details of fitting a quadratic; we just plug numbers into this formula and it gives us an answer. This makes Simpson’s rule almost as simple to use as the trapezoidal rule, and yet Simpson’s rule often gives much more accurate results.

Applying Simpson's rule involves dividing the domain of integration into many slices and using the rule to separately estimate the area under successive pairs of slices, then adding the estimates for all pairs to get the final answer: if, as before, we are integrating from x = a to x = b in slices of width h, then the three points bounding the first pair of slices fall at x = a, a + h and a + 2h, those bounding the second pair at a + 2h, a + 3h, a + 4h, and so forth. Then the approximate value of the entire integral is given by:

$$I(a,b) \simeq \tfrac{1}{3}h\left[f(a) + 4f(a+h) + f(a+2h)\right] + \tfrac{1}{3}h\left[f(a+2h) + 4f(a+3h) + f(a+4h)\right]$$

$$\ldots + \tfrac{1}{3}h\left[f(a+(N-2)h) + 4f(a+(N-1)h) + f(b)\right]$$

Note that the total number of slices must be even for this to work. Collecting terms together, we now have:

$$I(a,b) \simeq \tfrac{1}{3}h\left[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \ldots + f(b)\right]$$

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

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

Example 1:

Use Simpson's rule to calculate the integral of $x^4 - 2x + 1$ from x = 0 to x = 2 using, again, 10 slices. Compare the results to the output of the trapezoidal program.

Example 2:

a) Write a program to calculate E(x) for values of x from 0 to 3 in steps of 0.1. Choose for yourself what method you will use for performing the integral and a suitable number of slices.

$$E(x) = \int_0^x e^{-t^2} dt$$

b) When you are convinced your program is working, extend it further to make a graph of E(x) as a function of x.

Gaussian quadrature

The general form of the trapezoidal and Simpson rules is:

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

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

Suppose we are given a **nonuniform** set of N points x_k and we wish to create an integration rule of the form shown above that calculates integrals over a given interval from a to b, based only on the values $f(x_k)$ of the integrand at those points. In other words, we want to choose weights w_k so that the equation above works for general $f(x)$. To do this, we will fit a single polynomial through the values $f(x_k)$ and then integrate that polynomial from a to b to calculate an approximation to the true integral. To fit N points we need to use a polynomial of degree N − 1. The fitting can be done using the method of **interpolating polynomials**.

This is an interpolating polynomial of degree N-1:

$$\phi_k(x) = \prod_{m=1...N}^{m\neq k} \frac{(x-x_m)}{x_k-x_m}$$

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

where k varies from 1 to N, so the equation above defines N different polynomials. If we evaluate $\phi_k(x)$ at one sample point $x = x_m$, we get:

$$\phi_k(x_m) = \delta_{km}$$

where δ_{km} is the Kronecker delta.

Now consider the following expression:

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

If we evaluate it at any one of the sample points $x = x_m$ we get:

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

This means that $\Phi(x)$ is a polynomial of degree N-1 that fits the integrand f(x) at all of the sample points. Therefore:

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

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

Then,

$$w_k = \int_a^b \phi_k(x)dx$$

We have found a general method for creating an integration rule for any set of sample points x_k, we simply set the weights w_k equal to the integrals of the interpolating polynomials over the domain of integration. We may have to perform the integrals on the computer, using one of our other integration methods, such as Simpson’s rule. This may seem to defeat the point of our calculation, which was to find an integration method that didn’t rely on uniformly spaced sample points, and here we are using Simpson’s rule, which has uniformly spaced points. But in fact the exercise is not as self-defeating as it may appear. The important point to notice is that we only have to calculate the weights w_k once, and then we can use them to integrate as many different functions over the given integration domain as we like.

In fact, it's better than this. Once one has calculated the weights for a particular set of sample points and domain of integration, it's possible to map those weights and points onto any other domain without having to recalculate the weights. Typically one gives sample points and weights arranged in a standard interval, which for historical reasons is usually taken to be the interval from x = −1 to x = +1. Thus, to specify an integration rule one gives a set of sample points in the range $-1 \leq x_k \leq 1$ and a set of weights:

$$w_k = \int_{-1}^{1} \phi_k(x) dx$$

For mapping the points to a general domain that runs from x = a to x = b:

$$x'_k = \frac{1}{2}(b-a)x_k + \frac{1}{2}(b+a)$$

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

Once we have calculated the rescaled positions and weights then the integral itself is given by:

$$\int_a^b f(x)dx \simeq \sum_{k=1}^{N} w'_k f(x'_k).$$

To get an integration rule accurate up to the highest possible degree of 2N − 1, the sample points x_k should be chosen to coincide with the zeros of the Nth Legendre polynomial $P_N(x)$, and the corresponding weights w_k are:

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

This method is called Gaussian quadrature and although it might sound rather formidable from the description above, in practice it's beautifully simple: given the values x_k and w_k for your chosen N, all you have to do is rescale them if necessary and then perform the sum of the above equation in red.

The only catch is finding the values in the first place. In principle the results quoted above tell us everything we need to know but in practice the zeros of the Legendre polynomials are not trivial to compute.

Additional information:

A) Root finding

If $f'(x)$ is known analitically, the simplest and most common method to locate the roots of $f(x)$ is the Newton-Raphson method. This is an iterative method based on approximating the function by its tangent line, and finally computing the x-intercept of this tangent line. This x-intercept will typically be a better approximation to the original function's root than the first guess:

$$f'(x_i) = \frac{f(x_i)}{x_i - x_{i+1}}$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

B) Derivative of the Nth Legendre polynomial:

$$P'_N = \frac{N(P_{N-1} - xP_N)}{1 - x^2}$$

$$P_N(x) = \frac{(N+1)P_{N+1} + NP_{N-1}}{(2N+1)x}$$

In [ ]: