Integration

Introduction to numerical analysis

Riccardo Mannella

May 4, 2007

The problem of numerical integration can be solved with the help of ODE's: $\int_a^x f(y)dy = g(x)$ becomes the solution of

$$\frac{dg}{dx} = f(x)$$

with boundary $x_0 = a$.

The problem of numerical integration can be solved with the help of ODE's: $\int_a^x f(y)dy = g(x)$ becomes the solution of

$$\frac{dg}{dx} = f(x)$$

with boundary $x_0 = a$. It is however better to derive some general equations (think of how difficult it was to find the correct integration method for ODE's!).

The problem of numerical integration can be solved with the help of ODE's: $\int_a^x f(y)dy = g(x)$ becomes the solution of

$$\frac{dg}{dx} = f(x)$$

with boundary $x_0 = a$. It is however better to derive some general equations (think of how difficult it was to find the correct integration method for ODE's!).A generic algorithm has the structure:

$$\int_a^b f(x)dx = \sum w_i f(x_i)$$

where we can have two different cases: closed and open formulas.

The problem of numerical integration can be solved with the help of ODE's: $\int_a^x f(y)dy = g(x)$ becomes the solution of

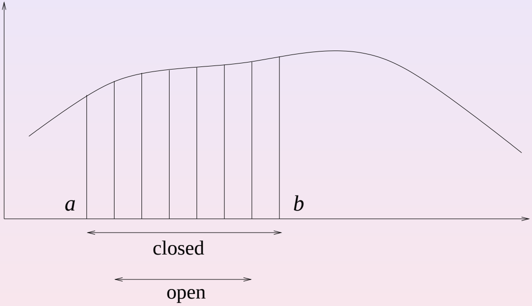
$$\frac{dg}{dx} = f(x)$$

with boundary $x_0 = a$. It is however better to derive some general equations (think of how difficult it was to find the correct integration method for ODE's!).A generic algorithm has the structure:

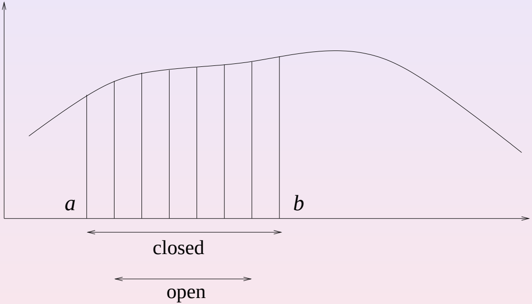
$$\int_a^b f(x)dx = \sum w_i f(x_i)$$

where we can have two different cases: closed and open formulas.In the following, $f_i = f(x_i)$, and typically $x_i = a + i * h$.

Closed formulas will use all the information up to a and b. Open formulas will not use the end point(s) a and/or b



Closed formulas will use all the information up to *a* and *b*. Open formulas will not use the end point(s) *a* and/or *b*



The main advantage of open formulas is that they can be used when the evaluation of the function at the end point(s) is ill defined, although the integral makes sense.

The working donkey of numerical integration is the trapezoidal rule:

$$\int_{x_1}^{x_2} f(x)dx = \frac{1}{2}h[f_1 + f_2] + O(h^3 f'')$$

It is exact for $f(x) = x$.

The working donkey of numerical integration is the trapezoidal rule:

$$\int_{x_1}^{x_2} f(x)dx = \frac{1}{2}h[f_1 + f_2] + O(h^3 f'')$$

It is exact for $f(x) = x$. It is worth mentioning how we get this relation: the polynomial which interpolates two points has the structure:

$$f(x) = f_1 + (f_2 - f_1) * x$$

and integrating $0 \leq x \leq 1$ we get the trapezoidal rule.

The working donkey of numerical integration is the trapezoidal rule:

$$\int_{x_1}^{x_2} f(x)dx = \frac{1}{2}h[f_1 + f_2] + O(h^3 f'')$$

It is exact for $f(x) = x$. It is worth mentioning how we get this relation: the polynomial which interpolates two points has the structure:

$$f(x) = f_1 + (f_2 - f_1) * x$$

and integrating $0 \leq x \leq 1$ we get the trapezoidal rule. For higher orders:

$$\int_{x_1}^{x_3} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + O(h^5 f^{(4)}) \quad \text{exact for } x^3!$$

$$\int_{x_1}^{x_5} f(x)dx = h\left[\frac{14}{45}f_1 + \frac{64}{45}f_2 + \frac{24}{45}f_3 + \frac{64}{45}f_4 + \frac{14}{45}f_5\right] + O(h^7 f^{(6)})$$

Easier to look at some relations:

$$\int_{x_0}^{x_1} f(x)\, dx = h[f_1] + O(h^2 f')$$

$$\int_{x_0}^{x_1} f(x)\, dx = h\left[\frac{3}{2}f_1 - \frac{1}{2}f_2\right] + O(h^3 f'')$$

Easier to look at some relations:

$$\int_{x_0}^{x_1} f(x)\, dx = h[f_1] + O(h^2 f')$$

$$\int_{x_0}^{x_1} f(x)\, dx = h\left[\frac{3}{2}f_1 - \frac{1}{2}f_2\right] + O(h^3 f'')$$

These relations are readily obtained through approximation and integration. The latter formula, for example, is obtained from $f(x) = f_1 + x(f_2 - f_1)$ as follows

$$\int_{-1}^{0} f(x)\, dx = -(-f_1) - \frac{(-1)^2}{2}(f_2 - f_1) = \left[\frac{3}{2}f_1 - \frac{1}{2}f_2\right]$$

Higher order formulas follow using higher order approximations.

Closed, extended interval

We are ready to integrate over extended intervals. From the trapezoidal rule,

$$\int_{x_1}^{x_2} f(x)\,dx = \frac{1}{2}h[f_1 + f_2] + O(h^3 f'')$$

we have

$$\int_{x_1}^{x_n} f(x)\,dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 .. + \frac{1}{2}f_n\right] + O((x_n - x_1)^3 f''/N^2)$$

Closed, extended interval

From the Simpson's rule,

$$\int_{x_1}^{x_3} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + O(h^5 f^{(4)})$$

we have

$$\int_{x_1}^{x_n} f(x)\,dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \right.$$
$$\left. \ldots + \frac{4}{3}f_{n-1} + \frac{1}{3}f_n\right] + O(1/N^4)$$

Open, extended interval

The idea is to combine the open formula for a single interval and a closed one for an extended interval. For example, combining:

$$\int_{x_0}^{x_1} f(x)\,dx = hf_1 + O(h^2 f')$$

and

$$\int_{x_1}^{x_n} f(x)\,dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 .. + \frac{1}{2}f_n\right] + O((x_n - x_1)^3 f''/N^2)$$

we have

$$\int_{x_0}^{x_n} f(x)\,dx = h\left[\frac{3}{2}f_1 + f_2 + f_3 .. + \frac{3}{2}f_{n-1}\right] + O(1/N^2)$$

Open, extended interval

From Simpson's extended rule

$$\int_{x_1}^{x_n} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \ldots + \frac{1}{3}f_n\right] + O(1/N^4)$$

and the open formula

$$\int_{x_0}^{x_1} f(x)\,dx = h\left[\frac{23}{12}f_1 - \frac{16}{12}f_2 + \frac{5}{12}f_3\right] + O(h^4 f^{(3)})$$

we have

$$\int_{x_0}^{x_n} f(x)\,dx = h\left[\frac{27}{12}f_1 + 0 + \frac{13}{12}f_3 + \frac{4}{3}f_4 + \ldots\right.$$
$$\left. + \frac{4}{3}f_{n-4} + \frac{13}{12}f_{n-3} + 0 + \frac{27}{12}f_{n-1}\right] + O(1/N^4)$$

The problem we have to face is: in practice, how many steps should we take?

The problem we have to face is: in practice, how many steps should we take? Suppose we use the trapezoidal rule as building block. The error associated with it will go like K/N^2.

The problem we have to face is: in practice, how many steps should we take? Suppose we use the trapezoidal rule as building block. The error associated with it will go like K/N^2. If we computed the integral doubling N, the error would decrease by a factor 4.

The problem we have to face is: in practice, how many steps should we take? Suppose we use the trapezoidal rule as building block. The error associated with it will go like K/N^2. If we computed the integral doubling N, the error would decrease by a factor 4. In any case, the error can be readily evaluated taking the difference between the integral evaluated with N steps (S_N) and the error evaluated with $2N$ steps (S_{2N}).

The problem we have to face is: in practice, how many steps should we take? Suppose we use the trapezoidal rule as building block. The error associated with it will go like K/N^2. If we computed the integral doubling N, the error would decrease by a factor 4. In any case, the error can be readily evaluated taking the difference between the integral evaluated with N steps (S_N) and the error evaluated with $2N$ steps (S_{2N}). We can actually do better if we wrote the exact relation for the trapezoidal rule!

Bernoulli's numbers

$$\int_{x_1}^{x_n} f(x)\,dx = h\left[\frac{1}{2}f_1 + f_2 + \ldots + \frac{1}{2}f_n\right]$$

$$-\frac{B_2 h^2}{2!}(f_n' - f_1') - \ldots - \frac{B_{2k}h^{2k}}{(2k)!}(f_n^{2k-1} - f_1^{2k-1}) - \ldots$$

The B's are Bernoulli numbers,

$$\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} B_n \frac{t^n}{n!}$$

The important message is that if N is doubled, the error goes down by 4. We can cancel the h^2 term if we used

$$S = \frac{4}{3}S_{2N} - \frac{1}{3}S_N$$

Romberg

The previous example is a way of obtaining an improved approximation through the evaluation of integrals done with a different number of mesh points, taking a suitable linear combination.

Romberg

The previous example is a way of obtaining an improved approximation through the evaluation of integrals done with a different number of mesh points, taking a suitable linear combination. A very elegant way of obtaining a better approximation is to carry on the subtraction: S has an error h^4, with known coefficients. Combining two S done with different N, we can futher reduce the error to terms h^6 and so on.

Romberg

The previous example is a way of obtaining an improved approximation through the evaluation of integrals done with a different number of mesh points, taking a suitable linear combination. A very elegant way of obtaining a better approximation is to carry on the subtraction: S has an error h^4, with known coefficients. Combining two S done with different N, we can futher reduce the error to terms h^6 and so on. Romberg's approach consists in computing the integral for a defined set of N, writing a rational expression as function of powers of $1/N$, and taking the limit of $N \to \infty$.

Romberg

The previous example is a way of obtaining an improved approximation through the evaluation of integrals done with a different number of mesh points, taking a suitable linear combination. A very elegant way of obtaining a better approximation is to carry on the subtraction: S has an error h^4, with known coefficients. Combining two S done with different N, we can futher reduce the error to terms h^6 and so on. Romberg's approach consists in computing the integral for a defined set of N, writing a rational expression as function of powers of $1/N$, and taking the limit of $N \to \infty$.Routines are available (see for instance Numerical Recipes) which implement the algorithm.

Gaussian quadratures use orthogonal polynomials to carry out the integration. The problem they solve is

$$\int f(x)W(x)\,dx = \sum_j w_j f(x_j)$$

where $W(x)$ is a measure ($W(x) > 0 \quad \int W(x)\,dx = 1$), and the x_j are not necessarily equally spaced.

Gaussian quadratures use orthogonal polynomials to carry out the integration. The problem they solve is

$$\int f(x)W(x)\,dx = \sum_j w_j f(x_j)$$

where $W(x)$ is a measure ($W(x) > 0 \quad \int W(x)\,dx = 1$), and the x_j are not necessarily equally spaced.Introduce the idea of functions product

$$\langle f|g\rangle \equiv \int W(x)f(x)g(x)\,dx$$

Orthogonal polynomials $p_k(x)$ are defined as

$$\begin{aligned} p_{-1}(x) &= 0 \\ p_0(x) &= 1 \\ p_{j+1}(x) &= (x - a_j)p_j(x) - b_j p_{j-1}(x) \end{aligned}$$

with

$$a_j \equiv \frac{\langle x p_j | p_j \rangle}{\langle p_j | p_j \rangle} \qquad b_j \equiv \frac{\langle p_j | p_j \rangle}{\langle p_{j-1} | p_{j-1} \rangle}$$

The j-th polynomial has j roots, interleaving the roots of the $j-1$-th polynomial. They are monic, and they can be normalised to form an orthonormal set.

Now, because the p_j are orthogonal, and $p_0(x) = 1$, it follows that, for virtually any set of x_j

$$\int W(x)p_0(x)\,dx = \sum_{j=1}^{N} w_j p_0(x_j) = 1$$

$$\int W(x)p_0(x)p_1(x)\,dx = 0 = \sum_{j=1}^{N} w_j p_1(x_j)$$

$$\dots$$

$$\int W(x)p_{N-1}(x)\,dx = 0 = \sum_{j=1}^{N} w_j p_{N-1}(x_j)$$

Assume that $f(x)$ is a polynomial at most of degree N: the relation

$$\int f(x)W(x)\,dx = \sum_{j=1}^{N} w_j f(x_j)$$

follows easily: $f(x)$ has N coefficients, the above equation is simply a mapping from the coefficient to a set of N unknown w_j, which can be easily computed once the x_j have been specified.

Assume that $f(x)$ is a polynomial at most of degree N: the relation

$$\int f(x)W(x)\,dx = \sum_{j=1}^{N} w_j f(x_j)$$

follows easily: $f(x)$ has N coefficients, the above equation is simply a mapping from the coefficient to a set of N unknown w_j, which can be easily computed once the x_j have been specified. The challenge is, however: can we find a set of crafted x_j such that the relation holds even when the degree of $f(x)$ is larger than N? The answer is “yes”, but we need to find the appropriate x_j.

Assume that $f(x)$ is a polynomial of at most $2N-1$ degree. It can be written, in general, as

$$f(x) = p_N(x)q_f(x) + r_f(x)$$

with $q_f(x)$ and $r_f(x)$ polynomials of degree less than N. Of course, we have

$$q_f(x) = \sum^{N-1} a_k p_k(x) \quad a_k = \frac{\langle p_k|q_f\rangle}{\langle p_k|p_k\rangle}$$

$$r_f(x) = \sum^{N-1} b_k p_k(x) \quad b_k = \frac{\langle p_k|r_f\rangle}{\langle p_k|p_k\rangle}$$

Now, the following holds:

$$\int W(x)f(x)dx = \int W(x)(p_N(x)q_f(x) + r_f(x))dx =$$
$$= \sum w_j(p_N(x_j)q_f(x_j) + r_f(x_j))$$

which becomes, if the x_j are the roots of p_N

$$\int W(x)f(x)dx = \sum w_j r_f(x_j) \equiv \int W(x)r_f(x)dx$$

But by hypothesis, r_f was of degree less than N, hence the integral above is exact!

We know that the x_j are the roots of p_N. What about the w_j? They can found as (this means we are using orthogonality to make the relation true for the set of basis polynomials)

$$\begin{bmatrix} p_0(x_1) & \dots & p_0(x_N) \\ p_1(x_1) & \dots & p_1(x_N) \\ \vdots & & \vdots \\ p_{N-1}(x_1) & \dots & p_{N-1}(x_N) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} \int W(x) p_0(x) dx \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

There is however a quicker way, based on an explicit expression,

$$w_j = \frac{\langle p_{N-1} | p_{N-1} \rangle}{p_{N-1}(x_j) p'_N(x_j)}$$

Time for some explicit cases:

$$\int_a^b W(x) f(x)\, dx = \sum_{i=1}^{N} w_j f(x_j)$$

(a,b)	$W(x)$	Recurrence	Name
$(-1,1)$	1	$(i+1)P_{i+1} = (2i+1)xP_i - iP_{i-1}$	Legendre
$(-1,1)$	$\frac{1}{\sqrt{1-x^2}}$	$T_{i+1} = 2xT_i - T_{i-1}$	Chebyshev
$(0,\infty)$	$x^c e^{-x}$	$(i+1)L_{i+1}^c = (-x+2i+c+1)L_i^c$ $-(i+c)L_{i-1}^c \quad c = 0, 1, \ldots$	Laguerre
$(-\infty,\infty)$	e^{-x^2}	$H_{i+1} = 2xH_i - 2iH_{i-1}$	Hermite

x_j roots of p_N, $w_j \equiv \frac{\langle p_{N-1} | p_{N-1} \rangle}{p_{N-1}(x_j) p'_N(x_j)}$

From Abramowitz Stegun, p.916-919, Gauss-Legendre:

n	x_j	w_j
2	± 0.577350269189626	1.0
3	± 0.774596669241483	0.555555555555556
	0.0	0.888888888888889
4	± 0.861136311594053	0.347854645137454
	± 0.339981043584856	0.652145154862546

The range (a, b) needs to be mapped into $(-1, 1)$: this is achieved as $y = 2(x-a)/(b-a) - 1$, which implies $x = a + (y+1)(b-a)/2$. We get:

$$\int_a^b f(x)\, dx = \frac{b-a}{2} \int_{-1}^{1} f(a + (y+1)(b-a)/2)\, dy$$

By improper integral we mean integrals where:

- The limiting value exists at one limit, but cannot be evaluated right at the limit, like $\sin(x)/x$
- one limit goes to infinite
- at either limit there is an integrable singularity (like $x^{-1/2}$ at $x = 0$)
- there is an integrable singularity inside the range of integration

The tools used are typically a change of variables and open formulas.

Case when either a or b diverge

Change the variables as

$$\int_a^b f(x)\,dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt \quad ab > 0$$

Of course the request $ab > 0$ means that we stay away from $x = 0$, and we can go through the transformation. Any integral routine can be used, and “infinite” means really “very large”.

Case when either a or b diverge

Change the variables as

$$\int_a^b f(x)\,dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt \quad ab > 0$$

Of course the request $ab > 0$ means that we stay away from $x = 0$, and we can go through the transformation. Any integral routine can be used, and "infinite" means really "very large". If $ab < 0$, split the integral into integrals where the integral containing zero is not transformed.

Case when at one limit the integrand diverges

Suppose that the integral has an integrable power-law singularity like $0 \leq \gamma < 1$ near a (ie. $f(x) \approx (x-a)^{-\gamma}$). Using the mapping $t = (x-a)^{1-\gamma}$ we have

$$\int_a^b f(x)\,dx = \frac{1}{1-\gamma}\int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(t^{\frac{1}{1-\gamma}} + a)\,dt \qquad b > a$$

Similarly if the singularity is at b:

$$\int_a^b f(x)\,dx = \frac{1}{1-\gamma}\int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(b - t^{\frac{1}{1-\gamma}})\,dt \qquad b > a$$

Alternatively, add and subtract a function with the same singularity and with known integral.

Case when the integrand diverges within a and b

Suppose the divergence is at $x = y$. There are two cases:

- the integrand is such that the divergence is integrable when restricted to (a, y) and (y, b). In this case, split the range in two, and use the prescription for the integration when the integrand diverges at one limit of integration.
- the divergence is not integrable on the two subranges, but the integral “makes sense”: this means that some cancellation is taking place, i.e. we are basically looking at the principal part of the integral: typically, rearrange the integrand so that the cancellation takes place in the numerics, as well.

Cauchy type singularity

An integral which appears often in physics is the integral

$$I(x) = \mathrm{P} \int_a^b \frac{f(x)}{x-y}\, dx$$

This can be handled in many ways (subtracting the singularity, choosing appropriate weighting functions etc.). An elegant way, which assumes $f(x)$ to be smooth along with first and second derivatives, uses integration by parts:

$$I(x) = \ln|x-y| f(x)|_a^b - \int_a^b \ln|x-y| f'(x)\, dx$$

If $f'(y) = 0$ we can compute the integral. Otherwise, integrate again by parts:

Cauchy type singularity

$$\begin{aligned} I(x) &= \ln|x-y| f(x)\Big|_a^b \\ &- \left[(x-y)\ln(x-y)-(x-y)\right] f'(x)\Big|_a^b \\ &+ \int_a^b \left[(x-y)\ln(x-y)-(x-y)\right] f''(x)\, dx \end{aligned}$$

Clearly, the integrand in the last term is now well behaved, unless $f''(y)$ has a discontinuity.

Open formulas

Any open formulas will do. In view of using something like Romberg's integration, a good candidate is the open formula:

$$\begin{aligned}\int_{x_1}^{x_n} f(x)\,dx &= h[f_{3/2}+f_{5/2}+\ldots+f_{n-3/2}+f_{n-1/2}]+\\ &\sum_{k=1} \frac{B_{2k}h^{2k}}{(2k)!}\left(1-2^{-2k+1}\right)\left(f_n^{2k-1}-f_1^{2k-1}\right)\end{aligned}$$

Unfortunately, halving the stepsize here does not help (we need to compute again all functions): however, tripling the steps help!