PY 421 - Introduction to Computational Physics

Lecture notes.

1 Algorithms for numerical integration.

We consider a function $f(x)$ defined over an interval of width 2δ which for convenience we take to be

$$-\delta \leq x \leq \delta \tag{1}$$

which is continuous and has a sufficient number of continuous derivatives over the interval. We would like to find an approximation formula which gives the value of

$$I = \int_{-\delta}^{\delta} f(x)\, dx \tag{2}$$

up to an error which is of the order of some power of δ. The formula must use the values of $f(x)$ at the end points and/or at some points inside the interval. The integral over a different range

$$I' = \int_{x_1}^{x_2} f(x)\, dx \tag{3}$$

will then be found by dividing the interval $x_1 \leq x \leq x_2$ in subintervals of width 2δ, applying the formula to each subinterval, and adding up the contributions from the various subintervals.

Let us consider first the case when we want to use the values of $f(x)$ at the end points $x = \pm\delta$. On general grounds we expect the formula to be linear in $f(\pm\delta)$ and the coefficients that multiply $f(\delta)$ and $f(-\delta)$ to be proportional to δ. Thus the formula will be

$$\int_{-\delta}^{\delta} f(x)\, dx \approx [af(-\delta) + bf(\delta)]\delta \tag{4}$$

with a and b constants to be determined.

Let us now notice the following. If we consider the Taylor series expansion of $f(x)$ around 0:

$$f(x) = f(0) + f'(0)x + \frac{1}{2}f''(0)x^2 + \frac{1}{6}f'''(0)x^3 + \frac{1}{24}f^{\text{iv}}(0)x^4 + \dots \tag{5}$$

it is obvious that the integral from $-\delta$ to δ of the term with x^k will produce a result which is proportional to $\delta^{(k+1)}$. So, in order for the formula to have an error $O(\delta^n)$ (i.e. of order δ^n), it must reproduce the correct integral of all powers x^k with $k \leq n-2$. (Equivalently, the first power where the formula can go wrong is x^{n-1}, since the integrals of the corresponding term and all higher terms in the power series expansion will contribute terms $O(\delta^n)$ or smaller to the integral.) We can therefore fix the constants a and b in Eq. 4 demanding that the formula be exact for as many powers of x: $x^0 = 1$, x, x^2 etc. as possible, given the freedom in the choice of the constants. In our particular case we have only two constants to set and thus we expect that we can impose only two conditions, which we find by taking $f(x) = x^0 = 1$ and $f(x) = x$, namely

$$[af(-\delta) + bf(\delta)]\delta = [a+b]\delta = \int_{-\delta}^{\delta} dx = 2\delta \tag{6}$$

with $f(x) = 1$ and

$$[af(-\delta) + bf(\delta)]\delta = [a(-\delta) + b\delta]\delta = \int_{-\delta}^{\delta} x\, dx = 0 \tag{7}$$

with $f(x) = x$. Equation 7 immediately gives $a = b$ and then Eq. 6 gives $a = b = 1$, so that the formula is

$$\int_{-\delta}^{\delta} f(x)\, dx \approx [f(-\delta) + f(\delta)]\delta \tag{8}$$

This is known as the **trapezoidal formula**. If we insert $f(x) = x^2$ in the formula we see that it no longer reproduces the correct integral:

$$[f(-\delta) + f(\delta)]\delta = [\delta^2 + \delta^2]\delta = 2\delta^3 \neq \int_{-\delta}^{\delta} x^2\, dx = \frac{4}{3}\delta^3 \tag{9}$$

and we conclude that the error in the formula is indeed of order δ^3.

We may decide to use only the value of the function at $x = 0$. In this case the integration formula will take the form

$$\int_{-\delta}^{\delta} f(x)\,dx \approx af(0)\delta \tag{10}$$

with only the constant a to be determined. We then fix a demanding that the formula reproduces correctly the integral of $x^0 = 1$ which gives us

$$a\delta = \int_{-\delta}^{\delta} dx = 2\delta \tag{11}$$

This fixes $a = 2$ and we get the formula

$$\int_{-\delta}^{\delta} f(x)\,dx \approx 2f(0)\delta \tag{12}$$

which is known as **mid-point based trapezoidal formula**.

In this particular case it so happens that the integral of $x^1 = x$ is also reproduced correctly

$$\int_{-\delta}^{\delta} x\,dx = 0 = 2 \times 0 \times \delta \tag{13}$$

Thus the error in this formula is $O(\delta^3)$, as with the trapezoidal formula.

If we use the values of the function at $x = \pm\delta$ and $x = 0$, then the integration formula will be

$$\int_{-\delta}^{\delta} f(x)\,dx \approx [af(-\delta) + bf(0) + cf(\delta)]\delta \tag{14}$$

Now we have three constants to play with and so we can demand that the integrals of $x^0 = 1, x$ and x^2 are reproduced correctly. This gives the conditions

$$(a + b + c)\delta = \int_{-\delta}^{\delta} dx = 2\delta \tag{15}$$

$$[a(-\delta) + c\delta]\delta = \int_{\delta}^{-\delta} x\,dx = 0 \tag{16}$$

$$[a\delta^2 + c\delta^2]\delta = \int_{-\delta}^{\delta} x^2\,dx = \frac{2}{3}\delta^3 \tag{17}$$

From Eq. 16 we get $c = a$. Then Eq. 17 gives $a = c = 1/3$ and Eq. 17 finally gives $b = 4/3$. Thus the integration formula is now

$$\int_{-\delta}^{\delta} f(x)\,dx \approx \left[\frac{1}{3}f(-\delta) + \frac{4}{3}f(0) + \frac{1}{3}f(\delta)\right]\delta \tag{18}$$

This is known as **Simpson's formula**.

In this case also we get one extra condition satisfied for free, since with $f(x) = x^3$ we have

$$\int_{-\delta}^{\delta} x^3\,dx = 0 = \left[\frac{1}{3}(-\delta)^3 + \frac{1}{3}\delta^3\right]\delta \tag{19}$$

Thus the error in this formula is $O(\delta^5)$.

Finally, we consider the case where we have the freedom of choosing the points where we evaluate $f(x)$ inside the integration interval. Guided by the symmetry in the previous formulae, we look now for a formula of the type

$$\int_{-\delta}^{\delta} f(x)\,dx \approx [af(-r\delta) + bf(0) + af(r\delta)]\delta \tag{20}$$

where $r \leq 1$ is, like a and b, a parameter which we will determine.

The symmetry in Eq. 20 guarantees that the formula will reproduce the correct value, namely 0, for the integral of all odd powers of x, since for odd n we have $a(-rx)^n + a(rx)^n = -a(rx)^n + a(rx)^n = 0$ in agreement with $\int_{-\delta}^{\delta} f(x)x^n\,dx = 0$ for odd n. Thus we need only demand that the formula reproduces the correct integral of as many even powers of x as possible. Since we have three parameters to play with, we may impose three conditions, namely that the formula be correct for $x^0 = 1$, x^2 and x^4. This gives the conditions

$$[a + b + a]\delta = \int_{-\delta}^{\delta} dx = 2\delta \tag{21}$$

$$[a(-r\delta)^2 + a(r\delta)^2]\delta = \int_{-\delta}^{\delta} x^2\,dx = \frac{2}{3}\delta^3 \tag{22}$$

$$[a(-r\delta)^4 + a(r\delta)^4]\delta = \int_{-\delta}^{\delta} x^4\,dx = \frac{2}{5}\delta^5 \tag{23}$$

Simplifying we get

$$2a + b = 2 \tag{24}$$

$$ar^2 = \frac{1}{3} \tag{25}$$

$$ar^4 = \frac{1}{5} \tag{26}$$

Dividing Eq. 26 by Eq. 25 we get $r^2 = 3/5$ or

$$r = \sqrt{\frac{3}{5}} = 0.774596669241483... \tag{27}$$

With this, Eqs. 25 and 24 immediately give

$$a = \frac{5}{9} \qquad b = \frac{8}{9} \tag{28}$$

so that the integration formula reads

$$\int_{-\delta}^{\delta} f(x)\, dx \approx \left[\frac{5}{9} f(-r\delta) + \frac{8}{9} f(0) + \frac{5}{9} f(r\delta)\right]\delta \tag{29}$$

This is known as the **Gaussian quadrature formula**.

About the error, since the formula also reproduces the correct integral of x^5 (equal to 0), the error will come from the terms of order x^6 and will be $O(\delta^7)$.

These formulae can now be used for the numerical integration over an interval of arbitrary length, by dividing the interval in subintervals of length 2δ, applying the formulae to the individual subintervals, and adding up the contributions. About the errors in the integration formulae, we should note that the errors coming from the individual subintervals will typically add, so that, if the error on a subinterval is $O(\Delta^n)$, the error in the approximation of the whole integral will be $O(\Delta^{n-1})$ since the number of subintervals is $O(1/\Delta)$.

In order to make connections to formulae which appear in the literature, we express the formulae in terms of the length of the subintervals, which we denote by Δ, rather than in terms of the length $\delta = \Delta/2$ of half the subintervals. Let us take the range of the integration to be $x_0 \leq x \leq x_N$ and imagine that this has been divided into N subintervals of length $\Delta = (x_N - x_0)/N$. It is convenient to introduce the notation

$$x_k = x_0 + k\Delta \tag{30}$$

with $k = 0, 1, \ldots N$, for the end-points of the intervals, and

$$x_{k+1/2} = x_0 + k\Delta + \frac{\Delta}{2} = x_k + \frac{\Delta}{2} \tag{31}$$

with $k = 0, 1, \ldots N-1$, for the mid-points of the subintervals. Then the integration formulae are as follows.

Trapeziodal formula:

$$\int_{x_0}^{x_N} f(x)\,dx = \left[\frac{1}{2}f(x_0)+f(x_1)+f(x_2)+\ldots+f(x_{N-1})+\frac{1}{2}f(x_0)\right]\Delta+O(\Delta^2) \tag{32}$$

Mid-point based trapeziodal formula:

$$\int_{x_0}^{x_N} f(x)\,dx = [f(x_{1/2})+f(x_{3/2})+\ldots+f(x_{N-1/2})]\Delta+O(\Delta^2) \tag{33}$$

Simpson's formula:

$$\begin{aligned}\int_{x_0}^{x_N} f(x)\,dx =\\ \left[\frac{1}{6}f(x_0)+\frac{2}{3}f(x_{1/2})+\frac{1}{3}f(x_1)+\frac{2}{3}f(x_{3/2})+\frac{1}{3}f(x_2)+\ldots\right.\\ \left.+\frac{1}{3}f(x_{N-1})+\frac{2}{3}f(x_{N-1/2})+\frac{1}{6}f(x_N)\right]\Delta+O(\Delta^4)\end{aligned} \tag{34}$$

Gaussian quadrature formula:

$$\begin{aligned}\int_{x_0}^{x_N} f(x)\,dx =\\ \left[\sum_{k=0}^{N-1}\left(\frac{5}{18}f(x_{k+1/2}-r\Delta/2)+\frac{4}{9}f(x_{k+1/2})+\frac{5}{18}f(x_{k+1/2}+r\Delta/2)\right)\right]\Delta\\ +O(\Delta^6)\end{aligned} \tag{35}$$

As a final remark, we note that the derivation of all these formulae rely on the fact that $f(x)$ is continuous with a sufficient number of continuous derivatives over the whole interval of integration. If this hypothesis does not hold the integration formulae may produce results which are much less accurate or, as for example in the case of an integrable singularity $f(x) \sim 1/\sqrt{(x)}$, some formulae may not be applicable at all.