PHYS527
Lecture 2: Calculus

- Numerical differentiation, central differences.
- Numerical integration:
  -Rules
  -Richardson's extrapolation
  -Improper integrals

Numerical differentiation:

The first topic we will discuss is how to handle derivatives numerically. We will assume that functions are represented in the computer as a table of pairs of numbers representing points of space x_n in one of the entries and $f(x_n)$ as the other entry. Recalling the definition of a derivative as the incremental quotient,

$$f(x)' = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

One is tempted to just represent numerically the derivative as,

$$f(x_n)' = \frac{f(x_{n+1})-f(x_n)}{x_{n+1}-x_n}$$

One can however, with the same computational cost, write better approximations to the derivative, and they are based on a simple observation: the above expression is a better approximation to the derivative at the **midpoint** of x_n and x_{n+1} than at each point.

To see this, let us consider the Taylor expansion

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2} f''(0) + \dots$$

And therefore

$$f(+h) = f(0) + hf'(0) + \frac{h^2}{2} f''(0) + \dots$$

$$f(-h) = f(0) - hf'(0) + \frac{h^2}{2} f''(0) + \dots$$

And,

$$\frac{f(h) - f(0)}{h} \approx f'(0) + O(h)$$

Whereas,

$$\frac{f(h) - f(-h)}{2h} \approx f'(0) + O(h^2)$$

That is, just by shifting the point where we are computing the derivative we gain a whole order in h with the same number of computations. This condenses the essence of differential calculus on a computer: use “centered” or “balanced” expressions for better results.

If you want higher accuracy you need to compute the function at more points,

$$f' \approx \frac{1}{12h}[f(-2h) - 8f(-h) + 8f(h) - f(2h)] + O(h^4)$$

And similar expressions for higher accuracies.

Should one go for higher accuracy? That largely depends on how expensive it is to compute the function. It is quite usual in physics to stick with second-order accuracy.

It is immediate to generalize all this for higher derivatives, for instance,

$$f'' \approx \frac{f'(h/2) - f'(-h/2)}{h} + O(h^2) \approx \frac{f(h) - 2f(0) + f(-h)}{h^2} + O(h^2)$$

And again, "symmetry" is crucial to good accuracy.

All these expressions are also true for partial derivatives. Functions of several variables are represented as a table with several entries, listing $x_n, y_n, \ldots, f(x_n, y_n, \ldots)$. We just have to repeat all above expressions variable by variable.

There are tables that give various approximations to derivatives, for instance in Abramowitz and Stegun.

One has to be careful with round-off error when computing derivatives. Normally this translates in not being too greedy with the value of h. That is, one has to make sure that x+h and x are numbers properly resolved when round error is taken into account. In practice this implies that h should not be too smaller than 10^{-4} or so than x.

Numerical integration:

To compute the integral $\int_a^b f(x)dx$

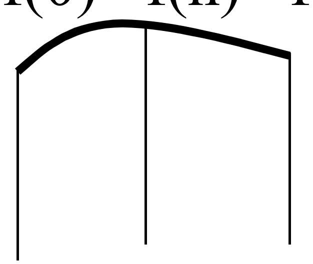
One partitions the a,b interval in N zones, $h = \frac{|b-a|}{N}$

And partitions the integral,

$$\int_a^b f(x)dx = \int_a^{a+2h} f(x)dx + \int_{a+2h}^{a+4h} f(x)dx + \ldots + \int_{b-2h}^{b} f(x)dx$$

One then approximates the integrals in the various intervals by approximating f(x) in the interval by an easy-to-integrate function. The simplest example is the trapezoidal rule,

f(0) f(h) f(2h)



$$\int_0^{2h} f(x)dx \approx \frac{h}{2}\left(f(0) + f(h) + f(h) + f(2h)\right) + O(h^3 f'')$$

To get a better formula, let us draw on our knowledge about discretized derivatives and write,

$$f(x) = f(0) + \frac{f(h) - f(-h)}{2h} x + \frac{f(h) - 2f(0) + f(h)}{h^2} \frac{x^2}{2} + \ldots$$

Integrating, we get

$$\int_{-h}^{h} f(x)dx = 2hf(0) + (f(h) - 2f(0) + f(h)) \frac{2h^3}{6h^2}$$

$$= \frac{h}{3}\left(f(h) + 4f(0) + f(-h)\right) + O(h^5 f^{iv})$$

Simpson's rule

If we now extend the above formulas to the whole domain of integration we get,

$$\text{Trapezoid}: \int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + \ldots f_{N-1} + \frac{1}{2}f_N\right] + O\left(\frac{(x_N - x_1)^3 f''}{N^2}\right)$$

$$\text{Simpson}: \int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 \ldots + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right]$$

$$+ O\left(\frac{f^{iv}}{N^4}\right)$$

Another way of getting higher order closed formulae and estimate errors:
Euler-MacLaurin formula:

$$E_n \equiv \int_{x_1}^{x_N} f(x)dx - h\left[\frac{1}{2}f_1 + f_2 + \ldots + \frac{1}{2}f_N\right] = \sum_{k=1}^{N} -\frac{B_{2k}h^{2k}}{(2k)!}\left(f_N{}^{(2k-1)} - f_1{}^{(2k-1)}\right)$$

$$+\frac{h^{2m+2}}{(2m+2)!}\int_{x_1}^{x_N} \overline{B}_{2m+2}\left(\frac{x-a}{h}\right) f^{(2m+2)}(x)dx$$

$$\overline{B}_j(x) = B_j(x)$$

Where B's are (gasp!) Bernoulli's numbers,

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

And B(x)'s are the extended Bernoulli's numbers,

$$\frac{t\, e^{xt}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(x) \frac{t^n}{n!}$$

Sketch of proof:

$$E_1 = \int_0^h f(x)dx - \frac{h}{2}\left[f(0)+f(h)\right] \qquad = \int_0^h f''(x)x(x-h)$$

Add and subtract $\displaystyle\int_0^h f''(x)\frac{h^2}{12}$

Ralston & Rabinowitz 1978

$$E_1 = -\frac{h^2}{12}\left[f'(h)-f'(0)\right]+\frac{1}{24}\int_0^h f^{iv}(x)x^2(x-h)^2\,dx$$

etc

The point of this formula is, however, very simple: the errors in the extended trapezoidal rule are even powers of h.

Therefore if I approximate an integral using N steps and obtain S_N, if I then go and approximate using 2N steps and obtain S_{2N}, the error in the latter approximation will be exactly 1/4 of the error in the first approximation. Therefore if I consider the combination,

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

It will cancel out the leading error contribution. The surviving error is of order $1/N^4$, exactly as in Simpson's rule. In fact, this approximation IS Simpson's rule, complete with the alternating 2/3 and 4/3 coefficients!

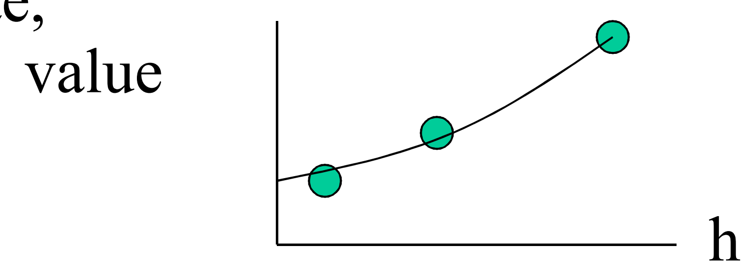
The neat way of viewing it in this perspective is that one clearly sees how would one go about generating higher order rules. And for the coefficients one needs Bernoulli's numbers.

Richardson's extrapolation:

("Archimedes the numerical analyst" 200BC
G. Phillips Am. Math. Mon. 88, 165 (1981))

The previous result is just an example (in the context of integration) of a powerful numerical technique known as Richardson's extrapolation. The gist of the technique is the following: if I know in detail how the leading error of a calculation depends on my discretization, I can cancel out such leading error by linear combination (or "extrapolation") of calculations with different values of the discretization parameter.

To put it a different way, any time I compute something using a discretization technique dependent on a parameter h, up to an error of $O(h^n)$, if I repeat the calculation for various values of h, I can "extrapolate" what the result would be in the limit h->0, which is what I want. The "extrapolation" will be better the more points I use to extrapolate,



The quite widely used Romberg integration algorithm just consists of applying k times the trapezoid rule and then perform a Richardson extrapolation,

```
      subroutine qromb(func,a,b,ss)
      parameter(eps=1.e-6,jmax=20,jmaxp=jmax+1,k=5,km=4)
      dimension s(jmaxp),h(jmaxp)
      h(1)=1.
      do 11 j=1,jmax
        call trapzd(func,a,b,s(j),j)
        if (j.ge.k) then
          l=j-km
          call polint(h(l),s(l),k,0.,ss,dss)
          if (abs(dss).lt.eps*abs(ss)) return
        endif
        s(j+1)=s(j)
        h(j+1)=0.25*h(j)
11    continue
      pause 'too many steps.'
      end
```

(implementation of Numerical Recipes)

Order vs. accuracy:

Should one go for the highest order method?

One should not get carried away. High order only translates itself into high accuracy if the function is “smooth enough” (it is well approximated by polynomials).

An extreme example would be to use a very high accuracy formula and try to get the integral evaluating the function at one point! Clearly this will work if the function is approximately constant.

If the features of your function are not properly resolved by the spacing chosen, no high order in 1/N will fix it.

Improper integrals:

- Integrand cannot be evaluated at one of the end-points, or at some mid-point (perhaps unknown).
- Integrand blows up at one of the end-points or at some mid-point.
- One (or both) of the integration limits is infinite.

One should distinguish improper from impossible. In all the above cases we are assuming that in spite of the apparent problem the integral exists. If the integral diverges, no numerical technique will cure it!

When the integrand blows up at one (or both) endpoints, but the integral is finite, the obvious answer is to obtain a formula for the integral that avoids evaluating the function at such points. For instance,

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{3}{2}f_2 + f_3 + f_4 + \ldots + f_{N-2} + \frac{3}{2}f_{N-1}\right] + O\left(\frac{1}{N^2}\right)$$

There are many such formulas, including ones that work for higher orders. How does one derive them? Write the right hand side as a linear polynomial in f_i with unknown coefficients. Then evaluate the formula for x, x^2, x^3, etc. and form a system of linear equations.

There does exist an Euler-MacLaurin theorem for open formulas, based on the “midpoint rule”,

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

$$+\frac{B_2 h^2}{4}\left(f'_N - f'_1\right) + \ldots + \frac{B_{2k} h^{2k}}{(2k)!}\left(1 - 2^{-2k+1}\right)\left(f_N{}^{(2k-1)} - f_1{}^{(2k-1)}\right)$$

And therefore one can Richardson-extrapolate and arrive at a Romberg formula for improper integrals of this kind.

Another obvious way to deal with an improper integral is to convert it to a proper one via a change of variables. Typical example is to map an infinite domain of integration into a finite one.

Example:

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

Which can be used for a>0 and b going to infinity or a going to minus infinity and b<0. (Otherwise you break it up into multiple integrals).

```
subroutine midinf(funk,aa,bb,s,n)
      func(x)=funk(1./x)/x**2
      b=1./aa
      a=1./bb
      if (n.eq.1) then
        s=(b-a)*func(0.5*(a+b))
        it=1
      else
        it=3**(n-2)
        tnm=it
        del=(b-a)/(3.*tnm)
        ddel=del+del
        x=a+0.5*del
        sum=0.
        do 11 j=1,it
          sum=sum+func(x)
          x=x+ddel
          sum=sum+func(x)
          x=x+del
11      continue
        s=(s+(b-a)*sum/tnm)/3.
        it=3*it
      endif
      return
```

From Numerical Recipes

When mapping an infinite domain of integration into a finite one, a concern that might appear is the following: one is considering the function at equally spaced intervals in the mapped domain. If one translates back into the original domain, as one approaches the limit of the domain the intervals between evaluations of functions become larger and larger.

To get a handle on this, one needs to demand that the features of the integrand be properly resolved by the chosen interval of evaluation in the compactified domain of integration. Otherwise one loses accuracy.

If the mapped function becomes "pathological" then the integral did not exist in the first place, e.g.

$$\int_3^\infty \sin(x)dx$$

There are many other identities one can use to handle divergent integrands. Let us mention only one more, useful when the integrand has power-law divergences at the endpoints,

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

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

Similar formulas can be found in math handbooks.

Summary

- Differentiation and integration: Taylor expand, evaluate. For higher orders, extrapolate.
- Richardson extrapolation: key to good numerical analysis.