Lecture 7

- Padé approximation.
- Monte Carlo method of integration.

Padé approximations:

A quotient of two polynomials:

$$R(x) \equiv \frac{\sum_{k=0}^{M} a_k x^k}{1 + \sum_{k=1}^{N} b_k x^k}$$

Is said to be a Padé approximation to a power series

$$f(x) = \sum_{k=0}^{\infty} c_k x^k$$

If f(0)=R(0) and,

$$\left.\frac{d^k}{dx^k} R(x)\right|_{x=0} = \left.\frac{d^k}{dx^k} f(x)\right|_{x=0}, \qquad k = 1, 2, \ldots, M+N$$

That is, the ratio R(x) has a power series expansion that agrees for the first M+N+1 coefficients with the power series expansion of f(x).

If one expands the above relation explicitly one gets a set of linear equations for the coefficients a_k and b_k as functions of the c's,

$$\sum_{m=1}^{N} b_m c_{N-m+k} = -c_{N+k}, \qquad k = 1, \ldots, N$$

(if M=N)

$$\sum_{m=0}^{k} b_m c_{k-m} = a_k, \qquad k = 1, \ldots, N$$

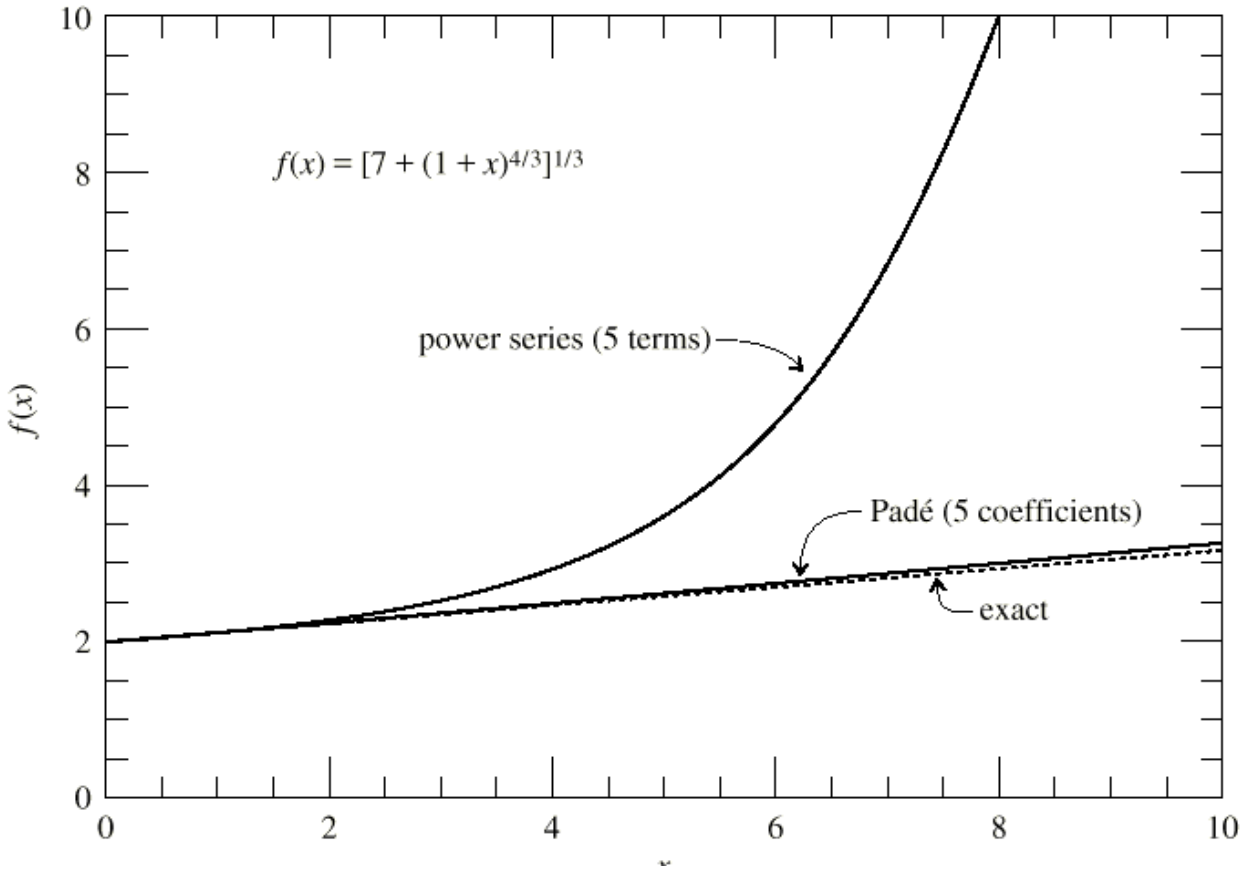
One first solves the first set for the b's, and then computes the a's through the second one. We will later in the course discuss methods to solve linear systems like these (Toeplitz matrices).

The power of the Padé approximation arises when the function considered has singularities. These can be non-obvious in the sense of being outside the domain in which one is considering the function, for instance they may occur somewhere in the complex plane even when one is considering the function only on real variables.

Example: $$f(x) = [7 + (1+x)^{4/3}]^{1/3}$$

This has a branch point in x=-1. The power series expansion is,

$$f(x) \approx 2 + \frac{1}{9}x + \frac{1}{81}x^2 - \frac{49}{8748}x^3 + \frac{175}{78732}x^4 + \cdots$$



And in the range shown diverges. The first five terms are therefore a bad approximation. The Padé approximation using the same five coefficients works much better.

Always? No!

Monte Carlo method of integration

As we have stated before in this course, the difficulty of evaluating multidimensional integrals grows very fast with the dimensionality. Yet in many physical applications (for instance statistical mechanics) one wishes to evaluate integrals that have very high dimensionality.

For instance, partition functions are integrals over the degrees of freedom of a system, so for N particles the integral is 3N dimensional. Moreover, the integrand is an exponential so it is quite peaked in given regions of the domain.

Moreover, a practical impediment to the kind of explicit integration methods we have covered is the fact that domains of integration in multidimensions can be quite complex to specify in an analytic form.

The Monte Carlo method deals with all of these issues by using a statistical sampling of the function to be integrated.

In its simplest incarnation, the method consists on evaluating,

$$I(f) = \int_V f(\vec{x}) d^n x = \frac{V}{N} \sum_{i=1}^{N} f(\vec{x}_i)$$

Where the x_i are randomly sprinkled points in the domain of integration. To handle irregular domains one simply sprinkles points in a hypercube containing the domain and sets the function to zero at points outside the desired domain. This can be easily handled with a conditional statement in the code. For highly irregular domains one should try something more elaborate since one wants to have as few “useless” points as possible.

As a rough estimate of the error of the integral, one can evaluate the standard-deviation error,

$$\text{Error} \approx V\sqrt{\frac{< f^2 > - < f >^2}{N}} \qquad < f >= \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)$$

This error estimate is only an indicator, since there is no guarantee that we are handling a Gaussian process. It is however, a quickly evaluated indicator.

The method would work perfectly for a constant function, and works better the smoother the function. We will see in a minute how we can improve the smoothness of the function to obtain the maximum efficiency from the method.

But first let us look at an example.

Domain of integration:

$$z^2 + \left(\sqrt{x^2+y^2} - 3\right)^2 \le 1$$

$$x \ge 1 \qquad y \ge -3$$

"Intersection of a donut with a box" (Numerical Recipes).

$$\rho \quad = \text{constant}$$

$$\int \rho \, dx\, dy\, dz \qquad \int x\rho \, dx\, dy\, dz \qquad \int y\rho \, dx\, dy\, dz \qquad \int z\rho \, dx\, dy\, dz \tag{7.6.5}$$

```
vol=3.*7.*2.                          Volume of the sampled region.
do 11 j=1,n
    x=1.+3.*ran2(idum)                Pick a point randomly in the sampled region.
    y=-3.+7.*ran2(idum)
    z=-1.+2.*ran2(idum)
    if (z**2+(sqrt(x**2+y**2)-3.)**2.le.1.)then      Is it in the torus?
        sw=sw+den                     If so, add to the various cumulants.
        swx=swx+x*den
        swy=swy+y*den
        swz=swz+z*den
        varw=varw+den**2
        varx=varx+(x*den)**2
        vary=vary+(y*den)**2
        varz=varz+(z*den)**2
    endif
enddo 11
w=vol*sw/n                            The values of the integrals (7.6.5),
x=vol*swx/n
y=vol*swy/n
z=vol*swz/n
dw=vol*sqrt((varw/n-(sw/n)**2)/n)     and their corresponding error estimates.
dx=vol*sqrt((varx/n-(swx/n)**2)/n)
dy=vol*sqrt((vary/n-(swy/n)**2)/n)
dz=vol*sqrt((varz/n-(swz/n)**2)/n)
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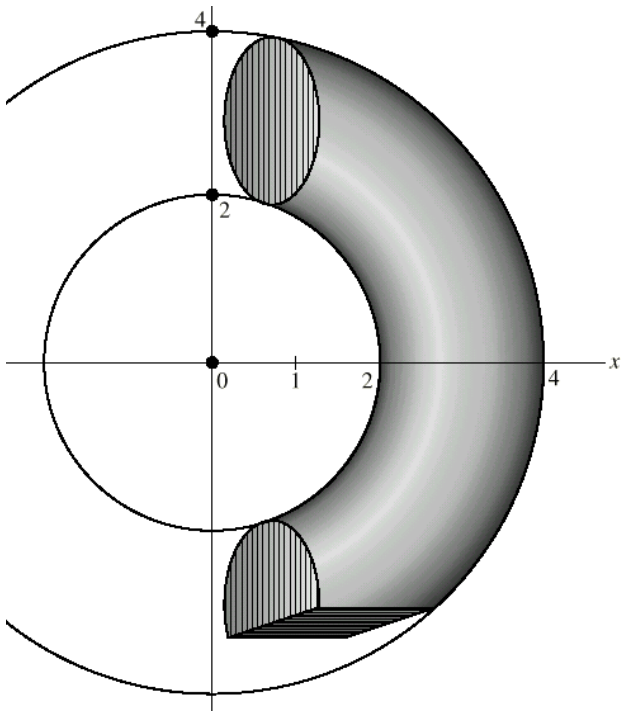

Suppose one wants to integrate a function that is harder to integrate in the sense that it varies rapidly in the domain of integration, say,

$$\rho(x, y, z) = e^{5z}$$

Just plugging this into the previous routine is a bad idea since points with lower values of z contribute almost nothing to the integral and are as "wasted" as points outside the domain. A better strategy is to change variables,

$$ds = e^{5z} dz \qquad \text{so that} \qquad s = \frac{1}{5} e^{5z}, \quad z = \frac{1}{5} \ln(5s)$$

Then $\rho\, dz = ds$ And we just change the limit of integration from $-1<z<1$ to $0.0135<s<29.682$

This was a bit miraculous. In general we will not be able to find a variable that brings the function to a constant. In such cases the tactic is to pull out a factor that makes the function as constant as possible.

A less obvious variation of the previous technique is called “importance sampling”. If we rewrite the change of variables strategy, one was doing,

$$\int f\,dV = \int (f/g)\,g dV = \int h\,g dV$$

One could evaluate this integral instead of sampling *hg* with uniform probability in the volume dV, by sampling h with probability density given by *gdV.*

In general given points sprinkled in the domain of integration with a probability p, appropriately normalized, $\int pdV = 1$

We can approximate the integral by,

$$I \equiv \int f\,dV = \int \frac{f}{p}\,pdV \approx \left\langle \frac{f}{p} \right\rangle \pm \sqrt{\frac{\langle f^2/p^2 \rangle - \langle f/p \rangle^2}{N}}$$

Another variation is called “stratified sampling”. Recall that the Monte Carlo evaluation of the integral is (up to the volume factor) equal to the mean of the function evaluated by the random sampling, and the variance was the error,

$$\langle f \rangle \equiv \frac{1}{N} \sum_i f(x_i)$$

If we now partition the interval into two sub-intervals a and b, each with N/2 points, another approximation to the integral could be,

$$\langle f \rangle' \equiv \frac{1}{2} \left(\langle f \rangle_a + \langle f \rangle_b \right)$$

The variance for such an approximation would be (exercise),

$$\mathrm{Var}\left(\langle f \rangle' \right) = \frac{1}{4} \left[\frac{\mathrm{Var}_a\left(f\right)}{N_a} + \frac{\mathrm{Var}_b\left(f\right)}{N - N_a} \right]$$

And this can be minimized if, $\frac{N_a}{N} = \frac{\sigma_a}{\sigma_a + \sigma_b}$

Sigma is square root of variance.

Which yields,

$$\mathrm{Var}\left(\langle f \rangle'\right) = \frac{\left(\sigma_a + \sigma_b\right)^2}{4N}$$

The interesting aspect of this result is that if any of the variances is lower than that of the whole interval, then one lowers the error. This is likely, since the variance should be lower if one is partitioning things in a finer way.

One should not get carried away: for instance if one partitions the volume in N sub-volumes, it would appear that the error instead of going as $N^{1/2}$ would go as N^{-1} and this would be a huge gain, which is unexpected. This is because this naïve argument does not take into account that in such case variances would be huge.

Summary

- Padé approximations handle better functions with singularities than Taylor series.
- The Monte Carlo method allows to compute higher dimensional integrals through a statistical sample.
- Various tricks depending on the function can be used.