Lecture 3

- Gaussian quadratures
- Multidimensional integrals

Gaussian quadratures:

Up to now we have considered integration formulas that are based on evaluating the function at pre-fixed points and choosing certain coefficients multiplying the functional values at those points.

What we will consider now is the possibility of not only choosing such coefficients but also choosing the points where to evaluate the function.

We therefore have at our disposal “twice” the number of degrees of freedom that we had before to construct a formula. We will not prove, but it is a rough guide that the formulas have twice the accuracy of the usual, regularly spaced ones.

The catch: as before, high order does not mean high accuracy in general. It is only true when the integrand is smooth enough in the sense of being well approximated by a polynomial.

So we are looking for formulae of the sort,

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

That become exact for polynomials of degree lower than N.

To construct formulae like these, we will start by considering Legendre polynomials (we will later see how to generalize this). Legendre polynomials $P_n(x)$ have the following properties,

- For each n, $P_n(x)$ is a polynomial of degree n.
- $\int_{-1}^{1} P(x)P_n(x) = 0$ if P(x) is a polynomial of degree less than n.

Roots of these polynomials lie in the interval -1,1 and as we'll see, they remarkably turn out to be good choices for x_i in the desired formula.

To see this, let us prove the following theorem:

If P(x) is any polynomial of degree less than 2n, then,

$$\int_a^b P(x)dx = \sum_{i=1}^{n} c_i P(x_i)$$

Where the x_i are the roots of the Legendre polynomials and,

$$c_i = \int_{-1}^{1} \prod_{j=1,\, j\neq i}^{n} \frac{x - x_i}{x_i - x_j} dx$$

Proof: let us start with the case of R(x) a polynomial of degree less than n. Let us rewrite R(x) through the Lagrange interpolating polynomial based at the n roots of the nth Legendre polynomial,

$$\int_{-1}^{1} R(x)dx = \int_{-1}^{1} \left[\sum_{i=1}^{n} \prod_{j=1,\, j\neq i}^{n} \frac{x - x_i}{x_i - x_j} R(x_i) \right] dx = \sum_{i=1}^{n} c_i R(x_i)$$

If we now consider a polynomial of degree less than 2n, one can divide it by the Legendre polynomial of degree n, producing two polynomials of degree less than n,

$$P(x) = Q(x)P_n(x) + R(x)$$

But since Q(x) is of degree less than n, then by the properties of the Legendre polynomials,

$$\int_{-1}^{1} Q(x)P_n(x) = 0$$

And since the x_i's are roots of the P_n,

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i)$$

We have,

$$\int_{-1}^{1} P(x)dx = \int_{-1}^{1} [Q(x)P_n(x) + R(x)]dx = \int_{-1}^{1} R(x)dx = \sum_{i=1}^{n} c_i R(x_i) \qquad \text{QED}$$

The roots of the Legendre polynomials are extensively tabulated, so are the coefficients c_i. One can look in tables and therefore find "formulae" for integration coming from Gauss quadratures rather similar to those we introduced for the trapezoid or Simpson's contructions.

An integral from a to b will have to be transformed, to use these formulae, into an integral from -1 to 1, which can be achieved through the change of variable,

$$t = \frac{2x - a - b}{b - a}$$

Which yields,

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{(b-a)t + (b+a)}{2}\right)\frac{(b-a)}{2}dt$$

From tables, n=2, x_1= 0.57735, c_1=1.0
x_2=-0.57735, c_2=1.0
n=3, x_1= 0.77459, c_1=0.55555
x_2= 0.0 , c_1=0.88888
x_3=-0.77459, c_3=0.55555

Example:

So say we want to evaluate, $\int_{1}^{1.5} e^{-x^2} dx$

First task is to transform it to the interval -1,1,

$$\int_{1}^{1.5} e^{-x^2} dx = \frac{1}{4}\int_{-1}^{1} e^{(-(t+5)^2/16)} dt$$

$$\mathrm{n}=2, \quad \int_{1}^{1.5} e^{-x^2} dx = \frac{1}{4}\left[1.0\times e^{-(5+0.577)^2/16} + 1.0\times e^{-(5-0.577)^2/16}\right] = 0.1094003$$

$$\mathrm{n}=3, \frac{1}{4}\left[0.5555\times e^{-(5+0.774)^2/16} + 0.5555\times e^{-(5-0.774)^2/16}\right]$$

$$+\frac{1}{4}\left[0.8888\times e^{-(5-0.0)^2/16}\right] = 0.1093642$$

It should be realized that in the previous proofs, we used little specifics about the Legendre polynomials, essentially that,

- For each n, $P_n(x)$ is a polynomial of degree n.
- $\int_{-1}^{1} P(x)P_n(x) = 0$ if P(x) is a polynomial of degree less than n.

These properties are shared by many other polynomials, especially if one chooses an inner product among them with a non-trivial weight function,

$$< f \mid g >= \int f(x)g(x)W(x)dx$$

Example: Chebyshev $W(x) = \sqrt{1-x^2}$ (Laguerre, Hermite, etc)

Using these polynomials is particularly effective for functions that are proportional to the weight function.

A direct (although not necessarily efficient) way of finding the weights is (as we argued in the case of equally spaced formulae), to solve the system of linear equations,

$$\begin{bmatrix} p_0(x_1) & \cdots & p_0(x_N) \\ \vdots & & \vdots \\ p_{N-1}(x_1) & \cdots & p_{N-1}(x_N) \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} \int_a^b p_0(x)dx \\ \vdots \\ \int_a^b p_{N-1}(x)dx \end{bmatrix}$$

So as before, the weights are the unknowns of a system of equations obtained by evaluating the proposed formula for the integrals of the elements of the basis of polynomials chosen.

In fact, one can see the more traditional formulas as particular cases of the ones we discussed here, for given polynomials.

The discussion of the errors in these formulae exceeds the scope of this course (and of most numerical analysis textbooks), but as we said, it is roughly (slightly less) than twice as good as that of equally spaced formulas.

But as we argued before, one should not get carried away with formal estimates of the error since order and accuracy are different things that depend on the particular function being integrated.

In practice what one does is to evaluate the integral with different orders of n and sees if the result is converging to the desired accuracy.

This is costly in the case of Gaussian quadratures since every time one increases the order, one needs to evaluate the function at different points. Methods that re-use the previous points are discussed in Numerical Recipes.

Multidimensional integrals

Are not easy…

If one simply tries to apply the previous methods for functions of several variables, one is hampered by the fact that the number of points that one needs to evaluate grows rapidly with the dimensionality of the integral.

Another factor that might complicate things is that the boundary of the region of integration might have a complicated shape.

If the boundary is complicated and low accuracy is tolerable, then the Monte Carlo method (we will discuss it later in this course) is the way to go. It is based on random samplings.

If the boundary is simple and the function is smooth, one can apply repeatedly the techniques we have discussed. One however, will have to rewrite the successive integrals in explicit form, e.g.,

$$I = \iiint dx\, dy\, dz\; f(x,y,z) = \int_{x_1}^{x_2} dx \int_{y_1(x)}^{y_2(x)} dy \int_{z_1(x,y)}^{z_2(x,y)} dz\; f(x,y,z)$$

And have at hand three different copies of the integration subroutine to avoid interference among them when called recursively.

If the integrand is strongly peaked in some region, and one knows the region, then one breaks up the integration domain treating the strongly peaked region separately.

If the integrand is strongly peaked in an unknown region, then one is pretty much out of luck, especially in higher dimensions.

Summary

- Gaussian quadratures “double” the accuracy by bringing in the evaluation point as an additional variable.
- Multidimensional integrals are hard.