LECTURE 19

Numerical Integration

Recall from Calculus I that a definite integral

$$\int_a^b f(x)dx$$

is generally thought of as representing the *area under the graph of* $f(x)$ *between the points* $x = a$ *and* $x = b$, even though this is actually only true when $f(x)$ is non-negative on $[a, b]$. However, the geometric interpretation of the derivative at least makes its the formal definition

$$\int_a^b f(x)dx \equiv \lim_{N\to\infty} \sum_{i=0}^{N} f(\tilde{x}_i)\Delta x \quad ; \quad \Delta x = \frac{b-a}{N} \quad , \quad \tilde{x}_i \in [a + i\Delta x, a + (i+1)\Delta x]$$

a little more palatable: for one thinks of the sum on the right hand side as a sum over the areas of a set of infinitesimal rectangles that just about cover the graph of $f(x)$.

Of course, in practice one never uses the limit definition to compute an integral. Rather, one relies on the Fundamental Theorem of Calculus, which says that

$$\int_a^b f(x)dx = F(b) - F(a)$$

where $F(x)$ is any function such that $\frac{dF}{dx} = f(x)$. Thus, the problem of carrying out a direct integral is reduced to finding an anti-derivative of the integrand.

However, there are many examples of functions f for which there is no closed formula for anti-derivative of f. A famous example is

$$f(x) = e^{x^2} .$$

Therefore, numerical integration is often the only means for ascribing values to expressions like

$$\int_0^1 e^{x^2} dx \quad .$$

Now just as in the case of the derivative, the formal definition leads naturally to simple numerical procedure. We simply choose a large value for N, set

$$\begin{aligned} \Delta x &= \frac{b-a}{N} \\ \tilde{x}_i &= a + \Delta x i + \frac{\Delta x}{2} \quad , \quad \text{the midpoint of the interval } [x_i, x_{i+1}] \end{aligned}$$

and calculate

$$\sum_{i=0}^{N} f(\tilde{x}_i)\Delta x \quad .$$

However, while it's easy to write this computational algorithm down, it's not so obvious how to figure out how accurate the resulting calculation will be for any given value of N.

In order to obtain a reliable estimate of the error we will replace the integrand $f(x)$ by a polynomial interpolation $P_f(x)$. The reason for doing this is two-fold. First of all, since $P_f(x)$ is a polynomial we can compute its integral exactly:

$$\int_a^b \left(\sum_{i=0}^n A_i x^i\right) dx = \sum_{i=0}^n (i+1) A_i (b^{i+1} - a^{i+1})$$

Secondly, we have an exact expression for the error that's introduced when we replace $f(x)$ by an n^{th} degree polynomial interpolation:

$$f(x) - P_f(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^n (x - x_i)$$

From this we can deduce

$$\int_a^b f(x)dx - \int_a^b P_f(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \int_a^b \left(\prod_{i=0}^n (x - x_i)\right)$$

Just as in the case of polynomial interpolation we would like to choose the interpolation nodes x_i in such a way that the factor

$$W = \int_a^b \left(\prod_{i=0}^n (x - x_i)\right) dx \equiv \int_a^b \omega(x) dx$$

is minimized. Recall that in the case of polynomial interpolation we discovered that the optimal choice of $n+1$ nodes x_i, at least on the interval $[-1,1]$ would be the roots of the Chebyshev polynomial $T_{n+1}(x)$. We have a similar situation here; however, instead of minimizing the maximal value of the product of the $(x - x_i)$'s we must instead try to minimize the integral of such a product. This leads us to using, instead of the roots of the ordinary Chebyshev polynomials, the roots of another special set of polynomials, the **Chebyshev polynomials of the second kind**. These polynomials are defined as follows:

$$U_n(x) = \frac{\sin\left((n+1)\cos^{-1}(x)\right)}{\sin\left(\cos^{-1}(x)\right)}$$

and have the following properties

- $U_n(x) = 2^{-n} x^n +$ lower order terms
- $2^{-n-1} U_{n+1}(x) = (x - x_0)(x - x_1)(x - x_2) \cdots (x - x_n)$ where
$$x_i = \cos\left(\frac{(i+1)\pi}{n+2}\right) \quad , \quad i = 0, 1, 2, \ldots, n$$
- If $x_0, \ldots, x_n$ are the roots of $U_{n+1}(x)$ then
$$\int_{-1}^1 \left|\prod_{i=0}^n (x - x_i)\right| dx = 2^{-(n+1)}$$
- If $\{\tilde{x}_i \mid i = 0, 1, \ldots, n\}$ is any other collection of $n+1$ point in $[-1,1]$, then
$$\int_{-1}^1 \left|\prod_{i=0}^n (x - \tilde{x}_i)\right| \geq 2^{-(n+1)}$$

Thus, one optimal technique for computing an integral

$$\int_{-1}^1 f(x)dx$$

would be to calculate an $n+1$ point interpolation $P_f(x)$ on the interval $[-1,1]$, using the points

$$x_i = \cos\left(\frac{(i+1)\pi}{n+2}\right) \quad , \quad i = 0, 1, 2, \ldots, n$$

as interpolation nodes and then setting

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} P_f(x)dx \quad .$$

To handle an integral over a more general interval, say $[a,b]$ we'd use the the same trick that we used for finding optimal nodes for ordinary interpolation; we just map the interval $[-1,1]$ linearly onto the interval $[a,b]$ and look to see where the the nodes of $U_n(x)$ land. Thus, we set

$$x_i = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{(i+1)\pi}{n+2}\right) \quad , \quad i = 0,1,2,\ldots,n$$

determine the interpolation polynomial $P_f(x)$ corresponding to this set of nodes, and finally set

$$\int_a^b f(x)dx = \int_a^b P_f(x)dx$$

PROBLEM 19.1. *Suppose*

$$\int_a^b f(x)dx$$

is calculated numerically by interpolating the function $f(x)$ at the points

$$x_i = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{(i+1)\pi}{n+2}\right) \quad , \quad i = 0,1,2,\ldots,n$$

and then integrating the interpolation polynomial between a and b. Express the maximal error in terms of a derivative of f, n, and the end points of integration a and b. (Hint: Write down a change of variables formula reduces the integral over $[a,b]$ to an integral over $[-1,1]$.)

1. Other Quadratures

Now actually the program outlined above can be bit too computer intensive. Certainly we can use up a lot of computer time finding the Newton form for the interpolation polynomial for a large set of nodes, converting the Newton form of the interpolation polynomial to standard form, and then integrating term by term. Often what suffices is a modest improvement over the naive algorithm coming from the formal definition of the Riemann integral.

Here's the basic idea. The formula

$$\int_a^b f(x) \approx \sum_{i=0}^{N} f(\tilde{x}_i)\Delta x \quad ; \quad \Delta x = \frac{b-a}{N} \quad , \quad \tilde{x}_i \in [a+i\Delta x, a+(i+1)\Delta x] \tag{19.1}$$

was based on the idea that the area under the graph of $f(x)$ can be approximated by forming a partitioning the interval $[a,b]$ into N subintervals $[x_i, x_{i+1}]$ of width Δx, approximating the area A_i under the graph of $f(x)$ under between x_i and x_{i+1} by

$$A_i \approx f(\tilde{x}_i)\,\Delta x \quad , \quad \tilde{x}_i \in [x_i, x_{i+1}] \tag{19.2}$$

and then summing over the contributions A_i. The idea we'll pursue now is how to improve the approximations (19.2).

Let's first note that the approximation (19.2) is about the worst possible. For effectively, we're replacing the function $f(x)$ by a 1 point polynomial interpolation of f on the interval $[x_i, x_{i+1}]$. No doubt our accuracy would improve if we instead used a three point polynomial interpolation instead.

For notational clarity, let's replace x_i and x_{i+1} by α and $x+2h$, and consider the Lagrange form of the three point interpolation of $f(x)$ on the interval $[\alpha, \alpha+2h]$ using the points $\alpha, \alpha+h, \alpha+2h$. We then have

(19.3)
$$f(x) \approx f(\alpha)\frac{(x-\alpha-h)(x-\alpha-2h)}{(-h)(-2h)} + f(\alpha+h)\frac{(x-\alpha)(x-\alpha-2h)}{(h)(-h)} + f(\alpha+2h)\frac{(x-\alpha)(x-\alpha-h)}{(2h)(h)}$$

The expresion on the right hand side is a second order polynomial in x. If we expand it in powers of x and integrate it between α and $\alpha+2h$ we obtain

$$\int_{\alpha}^{\alpha+2h} f(x)dx \approx \frac{h}{3}\left[f(\alpha)+4f(\alpha+h)+f(\alpha+2h)\right] \tag{19.4}$$

This formula is equivalent to **Simpson's Rule** (a rule that is often presented in elementary calculus courses.)

We can immediately apply this formula to get a new and improved version of (19.1). Setting

$$\alpha = x_i \quad , \quad h = \frac{\Delta x}{2}$$

we have

$$\int_{x_i}^{x_i+\Delta x} f(x) \approx \phi(x_i) = \frac{\Delta x}{2}\left[f(a)+4f(a+\Delta x/2)+f(a+\Delta x)\right]$$

and so, setting

$$\begin{aligned} \Delta x &= \frac{b-a}{2} \\ x_i &= a+i\Delta x \end{aligned}$$

we have

$$\int_a^b f(x)dx = \sum_{i=1}^{n}\int_{x_{i-1}}^{x_i} f(x)dx \approx \sum_{i=1}^{n}\phi\left(x_{i-1}\right)\Delta x$$

Of course, there's nothing stopping us from interpolating the subintervals $[x_i, x_{i+1}]$ at four, five or more points to obtain even more accurate quadrature formulae. However, the algebra between the analogs of equations (19.3) and (19.4) becomes pretty strenuous.

There is an easy way of guessing the correct quadature formula. To demonstrate this technique let me rework derivation of equation (19.4). The key idea is that polynomial interpolation at the points x_0, x_1, $\dots$, x_n will always produce a formula of the form

$$\int_a^b f(x)dx \approx \int\left(\sum_{i=0}^{n} f\left(x_i\right)\ell_i(x)\right)dx = \sum_{i=0}^{n} f\left(x_i\right)\int_a^b \ell_i(x)dx \tag{19.5}$$

where the $\ell_i(x)$ are the cardinal functions for the nodes $x_0, x_1, \dots, x_n$:

$$\ell_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n}\frac{(x-x_j)}{(x_i-x_j)}$$

If we define

$$A_i \equiv \int_a^b \ell_i(x)dx$$

then (**??**) takes the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} f\left(x_i\right)A_i \tag{19.6}$$

no matter what the function $f(x)$ is. Moreover, if $f(x)$ is a polynomial of degree less than or equal to n, then $f(x)$ is identical to its polynomial interpolation (recall that the error term is proprotional to $f^{(n+1)}(\xi)$ which would be zero if f were polynomial of degree $\leq n$). By taking $f(x) = 1, x, x^2, \dots, x^n$ we arrive at a series of $n+1$ equations for the $n+1$ constants A_i :

$$\begin{aligned}
b - a &= \int_a^b 1 dx = \sum_{i=0}^{n} A_i \\
\frac{1}{2}\left(b^2 - a^2\right) &= \int_a^b x dx = \sum_{i=0}^{n} x_i A_i \\
&\vdots \\
\frac{1}{n+1}\left(b^{n+1} - a^{n+1}\right) &= \int_a^b x^n dx = \sum_{i=0}^{n} x_i^n A_i
\end{aligned}$$

Solving this system of equations for the constants A_i will give us a quadature formula (19.6) that can be used for any function $f(x)$.

Let me now demonstrate this technique for the case where we do a three point interpolation to calculate

$$\int_a^{a+2h} f(x) dx \quad .$$

Set $x_0 = a$, $x_1 = a + h$, $x_2 = a + 2h$. The interpolation is exact when $f(x) = 1$. So

$$A_0 + A_1 + A_2 = \int_a^{a+2h} 1 dx = 2h$$

The interpolation is also exact when $f(x) = x$. So

$$A_0(a) + A_1(a+h) + A_2(a+2h) = \int_{a-2h}^{a+2h} x dx = \frac{1}{2}\left((a+2h)^2 - (a)^2\right) = 2ah - 2h^2$$

And the interpolation is exact when $f(x) = x^2$. Thus,

$$A_0(a)^2 + A_1(a+h)^2 + A_2(a+2h)^2 = \int_a^{a+2h} x^2 dx = \frac{1}{3}\left((a+2h)^3 - (a)^3\right) =$$

We thus arrive at the following system of equations

$$\begin{pmatrix} 1 & 1 & 1 \\ a & a+h & a+2h \\ a^2 & (a+h)^2 & (a+2h)^2 \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} 2h \\ \frac{1}{2}(a+2h)^2 - \frac{1}{2}a^2 \\ 2a^2 h + 4ah^2 + \frac{8}{3}h^3 \end{pmatrix}$$

The solution of this system

$$\begin{aligned}
A_0 &= \frac{1}{3}h \\
A_1 &= \frac{4}{3}h \\
A_2 &= \frac{1}{3}h
\end{aligned}$$

and so

$$\int_a^{a+2h} f(x) dx \quad \approx \frac{1}{3}hf(a) + \frac{4}{3}hf(a+h) + \frac{1}{3}hf(a+2h)$$

which is identical to (19.4).

Problem 19.2. *Find a quadrature formula for the integral*

$$\int_a^{a+3h} f(x)$$

corresponding to the case where the function $f(x)$ *is interpolated at four points:* $x_0 = a$*,* $x_1 = a + h$*,* $x_2 = a + 2h$*,* $x_3 = a + 3h$*;*