261: 4th April

Romberg Integration I

One of the themes of last term was interpolation. Given only a limited set of points, taken from a function, we saw that we could reconstruct the original function to a good approximation. We also saw that we could use the approximation to make an estimate of the integral of the original function.

This week, we shall lay the foundation for Romberg integration. This method is slightly more involved than those that we've already seen, but it has the benefit that the error analysis follow us the whole way through the calculation, so we can monitor our accuracy, at every step.

Romberg integration is an application of the Euler-MacLaurin summation formula, so before we look at integration itself, we must first look at this.

Euler-MacLaurin Summation Formula

Our starting point is to introduce the Bernoulli polynomials, which were developed by the brothers Jean and Jacques Bernoulli around 1700.

We can calculate them by integrating an arbitrary function $g(t)$. Now, although some of the step that follow may seem a bit arbitrary, we will stick with them because they will provide us with a systematic way of generating the Bernoulli polynomials.

We start by integrating $g(t)$

$$\int_0^1 g(t)dt = \int_0^1 1g(t)dt$$

Using integration by parts, we can integrate the 1 to get $t+c$, where c is a constant, whose value we will calculate later.

$$\begin{aligned}\int_0^1 1g(t)dt &= (t+c)g(t)\Big|_0^1 - \int_0^1 (t+c)\frac{dg(t)}{dt}dt \\ &= B_1(t)g(t)\Big|_0^1 - \int_0^1 B_1(t)\frac{dg(t)}{dt}dt\end{aligned}$$

$B_1(t) = t + c$ is the first Bernoulli function ($B_0(t)$ is taken to be 1). Integrating the second term gives

$$\int_0^1 B_1(t)\frac{dg(t)}{dt}dt = \frac{1}{2}B_2(t)\frac{dg(t)}{dt}\Big|_0^1 - \frac{1}{2}\int_0^1 B_2(t)\frac{d^2g(t)}{dt^2}dt$$

Analogously, we can generate the kth Bernoulli polynomial, from the $k-1$th, by using the equation

$$\int_0^1 B_{k-1}(t)\frac{d^{k-1}g(t)}{dt^{k-1}}dt = \frac{1}{k}B_k(t)\frac{d^{k-1}g(t)}{dt^{k-1}}\Big|_0^1 - \frac{1}{k}\int_0^1 B_k(t)\frac{d^kg(t)}{dt^k}dt$$

So, starting from $B_0(t) = 1$, we can generate the form of the subsequent Bernoulli polynomials, $B_1(t)$, $B_2(t)$, $B_3(t)$, etc. However, this only gives us the form of the Bernoulli polynomials. We still don't the values of the coefficients. We can calculate them with the following requirements: $B_{2l+1}(0) = 0$ and $B_{2l+1}(1) = 0$, where $l > 0$.

Let's use these expressions to work out the first few polynomials. We know that $B_0(t) = 1$ and that $B_1(t) = x + c$. Unfortunately, we can't use the two expressions to fix the value of c, because they only apply when $l > 0$ and for B_1, l would have to be 0. So we must take it on trust that $B_1(t) = t - \frac{1}{2}$.

To get $B_2(t)$, we integrate $B_1(t)$ and factor out $\frac{1}{2}$.

$$\int t - \frac{1}{2}dt = \frac{1}{2}t^2 - \frac{1}{2}t + c = \frac{1}{2}(t^2 - t + c)$$

So $B_2(t) = t^2 - t + c$. Similarly, integrating $B_2(t)$ gives

$$\int t^2 - t + c = \frac{1}{3}t^3 - \frac{1}{2}t^2 + ct + d$$

Factoring out $\frac{1}{3}$ gives

$$B_3(t) = t^3 - \frac{3}{2}t^2 + 3ct + d$$

Now we can use $B_3(0) = 0$ and $B_3(1) = 0$ to obtain values for c and d. $B_3(0) = 0$ implies that $d = 0$. Using $B_3(1) = 0$

$$B_3(1) = 1 - \frac{3}{2} + 3c$$

$$0 = -\frac{1}{2} + 3c$$

So $c = \frac{1}{6}$. This gives us for the second and third Bernoulli polynomials

$$B_2(t) = t^2 - t + \frac{1}{6}$$

$$B_3(t) = t^3 - \frac{3}{2}t^2 + \frac{1}{2}t$$

Question 1) Calculate $B_4(t)$ and $B_5(t)$.

Now let's return to the expression for $\int_0^1 g(t)dt$. We had

$$\int_0^1 g(t)dt = B_1(t)g(t)\Big|_0^1 - \int_0^1 B_1(t)\frac{dg(t)}{dt}dt$$

Evaluating $B_1(t)$ at 1 and 0, gives us

$$\int_0^1 g(t)dt = \frac{g(0)}{2} + \frac{g(1)}{2} - \int_0^1 B_1(t)\frac{dg(t)}{dt}dt$$

Using the relation between $B_{k-1}(t)$ to $B_k(t)$, we can substitute repeatedly for the integral of $B_1(t)$. If we do this m times, we get

$$\int_0^1 g(t)dt = \frac{g(0)}{2} + \frac{g(1)}{2} + \sum_{l=1}^{m} \frac{1}{l!} \left(B_l(0) \frac{d^{l-1}g(0)}{dt^{l-1}} - B_l(1) \frac{d^{l-1}g(1)}{dt^{l-1}} \right)$$

$$- \frac{1}{(m+1)!} \int_0^1 B_{m+1}(t) \frac{d^{m+1}g(t)}{dt^{m+1}} dt$$

We can use a few properties of the Bernoulli polynomials to simplify this. Firstly, we saw that $B_{2k+1}(0) = 0$ and $B_{2k+1}(1) = 0$, when $k > 0$. This means that the terms containing B_i where i is odd are 0. Secondly, when i is even, $B_i(0) = B_i(1)$. So if we label the value of $B_i(0) = B_i(1)$ as B_i and if we change the labels on the sums to reflect the fact that B_i with i odd are 0, we get

$$\int_0^1 g(t)dt = \frac{g(0)}{2} + \frac{g(1)}{2} + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!} \left(\frac{d^{2l-1}g(0)}{dt^{2l-1}} - \frac{d^{2l-1}g(1)}{dt^{2l-1}} \right)$$

$$- \frac{1}{(2m+1)!} \int_0^1 B_{2m+1}(t) \frac{d^{2m+1}g(t)}{dt^{2m+1}} dt$$

At this stage, it still isn't obvious how this result might be useful to us in an integration scheme. However, the two first terms are very similar to those that make up the trapezoidal sum, which we saw in the last tutorial.

The trapezoidal sum is an approximation to the area under a curve and looks like

$$T(h) = h \left(\frac{f(a)}{2} + f(a+h) + f(a+2h) + f(a+3h) + ... + f(b-h) + \frac{f(b)}{2} \right)$$

where the integral is between the limits a and b , N is the number of given points and $h = \frac{b-a}{N-1}$.

Rearranging our expression for the integral of $g(t)$, we get

$$\frac{g(0)}{2} + \frac{g(1)}{2} = \int_0^1 g(t)dt + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!} \left(\frac{d^{2l-1}g(1)}{dt^{2l-1}} - \frac{d^{2l-1}g(0)}{dt^{2l-1}} \right)$$

$$+ \frac{1}{(2m+1)!} \int_0^1 B_{2m+1}(t) \frac{d^{2m+1}g(t)}{dt^{2m+1}} dt$$

So far, our expression has been on the interval $[0, 1]$. If we obtain the same expressions for the intervals $[1, 2]$, $[2, 3]$ and so on, upto N, and add them up, we get

$$\frac{g(0)}{2} + g(1) + g(2) + ... + g(N-1) + \frac{g(N)}{2} = \int_0^N g(t)dt + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!} \left(\frac{d^{2l-1}g(N)}{dt^{2l-1}} - \frac{d^{2l-1}g(0)}{dt^{2l-1}} \right)$$

$$+ \frac{1}{(2m+1)!} \int_0^N B_{2m+1}(t) \frac{d^{2m+1}g(t)}{dt^{2m+1}} dt$$

This expression and the trapezoidal sum still aren't the same, although they are very similar. The difference is the presence of the h.

In our expression for the g, we have treated t as a dimensionless. However, in the trapezoidal sum, x is not. So, to obtain an expression for the sum, we need to replace the limits on $\int_0^N g(t)dt$ with b and a, where $b = Nh$. We also need to replace the derivatives in the sum. Instead of $\frac{d^{2l-1}g(t)}{dt^{2l-1}}$, we use $h^{2l-1}\frac{d^{2l-1}g(x)}{dx^{2l-1}}$. The trapezoidal rule becomes

$$h\left(\frac{g(a)}{2} + g(a+h) + g(a+2h) + ... + g(b-h) + \frac{g(b)}{2}\right) =$$

$$\int_a^b g(x)dx + \sum_{l=1}^{m} h^{2l}\frac{B_{2l}}{(2l)!}\left(\frac{d^{2l-1}g(b)}{dt^{2l-1}} - \frac{d^{2l-1}g(a)}{dt^{2l-1}}\right) + \frac{h^{2m+1}}{(2m+1)!}\int_a^b B_{2m+1}(x)\frac{d^{2m+1}g(x)}{dt^{2m+1}}dx$$

It is only at this stage that we can see why this formulation is useful. We now have the trapezoidal sum in terms a series in increasing order of h. This means that, if h is small, we can ignore the last term, which we still haven't evaluated. The benefit of ignoring the term is that we then have the trapezoidal sum on the left hand side, the value of the original integral on the right and side and then a sum, which gives the difference between them.

Before we finish this tutorial, we shall change the ignored term into a more commonly seen form. Integrating by parts gives

$$\frac{h^{2m+1}}{(2m+1)!}\int_a^b B_{2m+1}(x)\frac{d^{2m+1}g(x)}{dt^{2m+1}}dx =$$

$$\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}\left(B_{2m+2}(x)\frac{d^{2m+1}g(x)}{dx^{2m+1}}\bigg|_a^b - \int_a^b B_{2m+2}(x)\frac{d^{2m+2}g(x)}{dx^{2m+2}}\right)$$

We subtract $\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}B_{2m+2}\frac{d^{2m+1}g(x)}{dx^{2m+1}}\bigg|_a^b$ from the first term on the right hand side. To the second, we add its equivalent, $\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}\int_a^b B_{2m+2}\frac{d^{2m+2}g(x)}{dx^{2m+2}}dx$. This gives

$$\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}\left[(B_{2m+2}(t) - B_{2m+2})\frac{d^{2m+1}g(t)}{dx^{2m+1}}\bigg|_0^1 - \int_a^b (B_{2m+2}(t) - B_{2m+2})\frac{d^{2m+2}g(x)}{dx^{2m+2}}dx\right]$$

The first term is zero, because $B_{2m+2} = B_{2m+2}(0) = B_{2m+2}(1)$. For the second term, we can find a value of ξ, where $a < \xi < b$, so that it takes the following form

$$-\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}\int_a^b (B_{2m+2}(t) - B_{2m+2})\frac{d^{2m+2}g(x)}{dx^{2m+2}}dx =$$

$$-\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}\int_a^b (B_{2m+2}(t) - B_{2m+2})\,dx\frac{d^{2m+2}g(\xi)}{dx^{2m+2}}$$

In this case, $\int_a^b B_{2m+2}(x)dx = 0$, making it equal to

$$\frac{h^{2m+1}}{(2m+1)!}\frac{1}{2m+2}B_{2m+2}\frac{d^{2m+2}g(\xi)}{dx^{2m+2}}$$

$$= \frac{h^{2m+1}}{(2m+2)!} B_{2m+2} \frac{d^{2m+2} g(\xi)}{dx^{2m+2}}$$

Question 2) a) If $a = 0$, $b = 1$, $N = 3$, $m = 1$ and $g = \frac{x^5}{5} + x^3 + 2$, calculate the value of

$$\frac{h^{2m+1}}{(2m+1)!} \int_a^b B_{2m+1}(x) \frac{d^{2m+1} g(x)}{dt^{2m+1}} dx =$$

b) Equating this with,

$$= \frac{h^{2m+1}}{(2m+2)!} B_{2m+2} \frac{d^{2m+2} g(\xi)}{dx^{2m+2}}$$

Calculate the value of ξ.