APPM 1350: Section 4.9: Numerical Integration

So long as $f(x)$ is piecewise continuous on $[a,b]$, then the definite integral

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

exists in the sense of having a numerical value. However, it is not always possible to evaluate the integral analytically. For example;

$$\int_0^{\pi/2} \sqrt{1-\tfrac{1}{2}\cos^2 t}\;dt$$

is what is known as an elliptic integral. The function $\sqrt{1-\frac{1}{2}\cos^2 t}$ is continuous on $[0,\pi/2]$ and positive, so the integral clearly has a numerical value equal to the area under the curve. However, the antiderivative of the integrand cannot be expressed in terms of elementary functions. Hence we cannot use the fundamental theorem of calculus to evaluate this integral.

In cases such as this we resort to <u>numerical integration</u> or <u>numerical quadrature</u>. This means approximating the value of the integral using some appropriate summation technique. The simplest of these are the Riemann sums where for a n-subinterval partition of $[a,b]$ we have

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{n} f(c_k)\,\Delta x_k$$

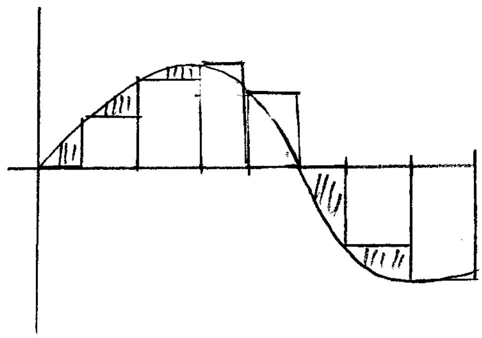
where

$$a = x_0 < x_1 < \cdots < x_n = b$$

$$\Delta x_k = x_k - x_{k-1}$$

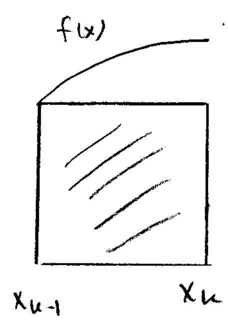
$$c_k \in [x_{k-1}, x_k]$$

However, especially for small n, this method (also called the rectangle rule) is often not very accurate as illustrated by the diagram below:



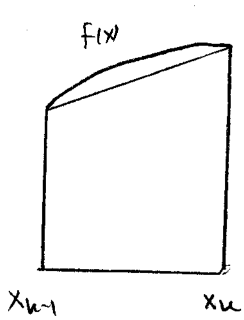
The Trapezoidal Rule

The rectangle rule gives poor results because a constant is usually a poor approximation to a function over a finite subinterval. So to improve our approximation, let's try a function that better approximates the function. We started with a constant, an obvious next step is to try a straight line (a constant is a 0th order polynomial, a straight line is a 1st order polynomial, so we are using polynomial approximations to $f(x)$ here). So over some subinterval, instead of



$$\text{Area} \approx f(x_{k-1})(x_k - x_{k-1})$$

we try:



$$\text{Area} \approx \frac{f(x_{k-1}) + f(x_k)}{2}(x_k - x_{k-1})$$

So our approximation to the definite integral becomes

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{n} \frac{f(x_{k-1}) + f(x_k)}{2} \Delta x_k$$

If we use equal subintervals this yields what is known as the <u>trapezoidal rule</u> because inside of summing the areas of rectangles we are now summing the area of trapezoids.

<u>The Trapezoidal Rule</u>

To approximate $\int_a^b f(x)\,dx$, use

$$T = \frac{h}{2}\left(y_0 + 2y_1 + \cdots + 2y_{n-1} + y_n\right)$$

for n subintervals of length $h = \frac{b-a}{n}$ and $y_k = f(x_k)$

The values of 2 appear because the value $f(x_k)$ shows up in the area of the trapezoid for $[x_{k-1}, x_k]$ and for $[x_k, x_{k+1}]$. No such double counting occurs at the endpoints, hence there is no factor of two at either end of the series.

The error of this approximation is

$$\boxed{E_T = \int_a^b f(x)\,dx - T}$$

It is shown in advanced calculus that

If f'' is continuous and M is <u>any</u> upper bound of $|f''|$ on $[a,b]$, then

$$|E_T| \leq \frac{b-a}{12} h^2 M$$

Example

Use the trapezoidal rule with $n = 10$ to approximate $\int_0^1 x^3\,dx$

Solution:

Partition $[0,1]$ into 10 subintervals of length

$$h = \frac{1.0}{10} = 0.1$$

Note that

$$x_k = kh \qquad (k = 0, \dots, 10)$$

Then from the trapezoidal rule;

$$\int_0^1 x^3\,dx = \frac{1}{20}(y_0 + 2y_1 + \dots + 2y_9 + y_{10})$$

$$= \frac{1}{20}\left[y_0 + y_{10} + 2\sum_{k=1}^{9} y_k \right]$$

$$= \frac{1}{20}\left[1 + 2\sum_{k=1}^{9} k^3 (0.1)^3 \right] \qquad \text{since } y_0 = (0)^3 \text{ \& } y_{10} = (1)$$

$$= \frac{1}{20}\left[1 + \frac{1}{500}\sum_{k=1}^{9} k^3 \right]$$

$$= \frac{1}{20}\left[1 + \frac{1}{500}\left[\frac{9(10)}{2}\right]^2 \right] \qquad \text{from eq 3, page 311}$$

$$= \frac{1}{20}\left[1 + \frac{81}{20} \right]$$

$$= 0.2525$$

The exact value is of course $1/4$. So the error is

$$E_T = 0.25 - 0.2525 = 0.0025$$

So the trapezoidal rule with 10 subintervals is accurate to

$$\frac{0.0025}{0.25} \times 100 = 1\%$$

Note, in this case we know the error. But suppose we didn't? Then we can estimate it using

$$|E_T| \leq \frac{b-a}{12} h^2 M$$

where

$$M \geq \max_{x \in [a,b]} |f''(x)|$$

In our case:

$$f'(x) = 3x^2$$
$$f''(x) = 6x$$

$$\Rightarrow \max_{x \in [0,1]} |f''(x)| = 6$$

Using $M = 6$, then

$$|E_T| \leq \frac{1}{12}\left(\frac{1}{10}\right)^2 6 = 0.005$$

This bound on the error is in this case twice the true error (2% versus 1%)

Note that the bound on the error $|E_T|$ can be used to estimate how many subintervals are necessary to guarantee a particular accuracy Erequired, then

(Erequired > 0)

$$|E_T| \leq \frac{b-a}{12} h^2 M \leq E_{required}$$

$$\Rightarrow |E_T| \leq \frac{(b-a)}{12} \left(\frac{b-a}{n}\right)^2 M \leq E_{required}$$

$$\Rightarrow |E_T| \leq \frac{(b-a)^3}{12} M \left(\frac{1}{n}\right)^2 \leq E_{required}$$

Hence

$$\frac{(b-a)^3}{12} \frac{M}{n^2} \leq E_{required}$$

$$\Rightarrow n \geq \sqrt{\frac{(b-a)^3 M}{12\, E_{required}}}$$

So using our previous example, $M = \max_{x \in [0,1]} |f''(x)| = 6$ and $b - a = 1$, to guarantee an absolute error less than or equal to 10^{-4} would require

$$n \geq \sqrt{\frac{6}{12 \times 10^{-4}}} = \frac{100}{\sqrt{2}} = 70.7 \, .$$

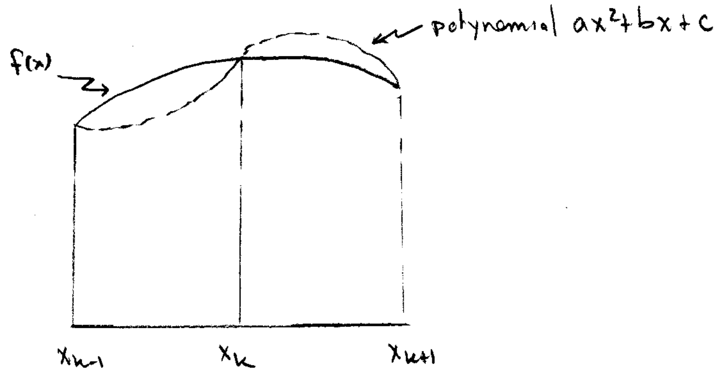
So $n = 71$ subintervals would suffice.

Simpson's Rule

As mentioned before, the rectangle rule uses a constant which is a 0th order polynomial. The trapezoidal rule, which is more accurate, uses a linear function to approximate the curve. This is a 1st order polynomial. Simpson's rule goes one order up and uses a quadratic equation to approximate the function f(x) on subintervals in order to estimate the definite integral

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

In particular, consider two adjacent subintervals



The idea is to approximate f(x) on $[x_{k-1}, x_{k+1}]$

$$g(x) = ax^2+bx+c$$

To determine a, b, and c, define $y_k = f(x_k)$ and note that

$$y_{k-1} = a x_{k-1}^2 + b x_{k-1} + c$$

$$y_k = a x_k^2 + b x_k + c$$

$$y_{k+1} = a x_{k+1}^2 + b x_k + c$$

These three equations can be solved for a, b, and c. The area approximated by the quadratic over $[x_{k-1}, x_{k+1}]$ is then:

$$A_k = \int_{x_{k-1}}^{x_{k+1}} (ax^2+bx+c)\,dx$$

$$= \frac{a}{3}x^3 + \frac{b}{2}x + cx \Bigg|_{x_{k-1}}^{x_{k+1}}$$

Evaluating this and substituting in a, b, and c, we get (see appendix A.4 on page A-17 of thomas):

$$A_k = \frac{h}{3}\left(y_{k-1} + 4y_k + y_{k+1}\right)$$

So now, partition $[a,b]$ into n subintervals where n is even. Approximate $f(x)$ on each $[x_{k-1}, x_{k+1}]$, $k = 1, 3, 5, \ldots, n-1$ with a quadratic whose definite integral is A_k. The approximate definite integral is then

$$\int_a^b f(x)\,dx \approx A_1 + A_3 + \cdots + A_{n-1}$$

This is Simpson's rule. Expanding the A_k's we get

Simpson's rule

To approximate $\int_a^b f(x)\,dx$ use

$$S = \frac{h}{3}\left(y_0 + 4y_1 + 2y_2 + 4y_3 + \cdots + 2y_{n-2} + 4y_{n-1} + y_n\right)$$

The y's are the values of f at the partition points (i.e., $y_k = f(x_k)$)

$$x_k = a + kh$$

where

$$h = \frac{b-a}{n}$$

and n is even.

Again, it is shown in advanced calculus that

> If $f^{(4)}$ is continuous and M is any upper bound for the values of $|f^{(4)}|$ on $[a,b]$, then
>
> $$|E_S| \leq \frac{b-a}{180} h^4 M$$
>
> where
>
> $$E_S = \int_a^b f(x)dx - S$$

Example

Apply Simpson's rule with $n=4$ to approximate $\int_0^1 x^4\,dx$

Solution:

If $n=4$, then $\frac{b-a}{n} = \frac{1}{4}$

and

$$\begin{aligned} x_0 &= 0 & & y_0 = 0 \\ x_1 &= 1/4 & & y_1 = (1/4)^4 \\ x_2 &= 1/2 & \Rightarrow \quad & y_2 = (1/2)^4 \\ x_3 &= 3/4 & & y_3 = (3/4)^4 \\ x_4 &= 1 & & y_4 = 1 \end{aligned}$$

Then

$$S = \frac{1}{12}\left(0 + 4\left(\tfrac{1}{4}\right)^4 + 2\left(\tfrac{1}{2}\right)^4 + 4\left(\tfrac{3}{4}\right)^4 + 1\right)$$

$$= \frac{154}{768}$$

$$\approx 0.2005$$

The exact result is 0.2, so the $n=4$ quadrature is exact to within 2.5%

Trapezoidal -vs- Simpson's Rule

Notice that the error bound for the trapezoidal rule is proportional to h^2 while it is proportional to h^4 for Simpson's rule. We say that the error is order of h^2, written $O(h^2)$, for the trapezoidal rule and order h^4 (i.e., $O(h^4)$) for Simpson's rule. Since $h^2 > h^4$ for $0 < h < 1$, Simpson's rule is generally the more accurate of the two. However, there are exceptions, for example when $f(x)$ is a linear function both techniques are exact and hence have the same error (zero in this special case). But as a rule, Simpson's will be the more exact quadrature technique.