

Lecture 12: Numerical Integration

See pictures of numerical integration courtesy of Eric Shea-Brown.

Numerical integration calculates the area under a given curve using a numerical approximation. The most basic methods are inspired by the definition of integration of a function $f(x)$ defined on an interval $[a, b]$:

$$\int_a^b f(x)dx = \lim_{h \rightarrow 0} \sum_{j=0}^n f(x_j)h$$

where $b - a = nh$.

If we consider the sum for a fixed h rather than in the theoretical limit as h goes to zero, then as h becomes smaller the summation approximation becomes more accurate and this would be one method of numerical integration, otherwise called quadrature.

A general quadrature formula looks like this:

$$Q[f] = \sum_{j=0}^n w_j f(x_j) = w_0 f(x_0) + \dots + w_n f(x_n)$$

where $a = x_0 < x_1 < x_2 < \dots < x_n = b$.

If we approximate the integral with such a quadrature formula we have an associated error with the approximation (as we did with the numerical differentiation).

$$\int_a^b f(x) dx = Q[f] + E(f)$$

Newton-Cotes Formulas We begin by assuming that the function $f(x)$ can be approximated by a polynomial

$$P_n(x) = \sum_{j=0}^n a_j x^j$$

where the truncation error in this case would be proportional to the $(n + 1)^{th}$ derivative

$$E(f) = A f^{(n+1)}(c)$$

where A is constant. Given

$$x_j = x_0 + hj \quad f_j = f(x_j)$$

We are able to then obtain several integration algorithms.

The Trapezoidal, Simpson's and Simpson's 3/8 rules are:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12}f''(c)$$

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90}f^{(4)}(c)$$

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80}f^{(4)}(c)$$

There are several ways of deriving these methods, lets derive the trapezoid method here (see Kutz's notes for derivation of Simpson's rule).

A geometrical approach is as follows:

$$\begin{aligned}\int_{x_0}^{x_1} &= \approx \text{area of trapezoid} \\ &= \frac{1}{2}(f(x_1) + f(x_0))(x_1 - x_0) \\ &= (x_1 - x_0)\frac{f(x_0) + f(x_1)}{2}\end{aligned}$$

Derivation of the trapezoidal rule from Calculus beginning with the polynomial approximation to the function $f(x)$

$$f(x) \approx f_n(x) = \sum_{j=0}^n a_j x^j$$

where $f_n(x)$ is the n^{th} order polynomial. The Trapezoidal method assumes $n = 1$:

$$\begin{aligned} \int_{x_0}^{x_1} f(x) dx &= \int_{x_0}^{x_1} f_1(x) dx + E \\ &= \int_{x_0}^{x_1} \sum_{j=0}^1 a_j x^j dx + E(f) \\ &= \int_{x_0}^{x_1} (a_0 + a_1 x) dx + E(f) \\ &= a_0(x_1 - x_0) + a_1 \left(\frac{x_1^2 - x_0^2}{2} \right) + E(f) \end{aligned}$$

Now inserting the endpoint values

$$\begin{aligned}f(x_0) &= a_0 + a_1x_0 \\f(x_1) &= a_0 + a_1x_1\end{aligned}$$

Solving for a_1 and a_2 :

$$\begin{aligned}a_1 &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} \\a_0 &= \frac{f(x_0)x_1 - f(x_1)x_0}{x_1 - x_0}\end{aligned}$$

Replacing a_0 and a_1 results in the Trapezoidal formula:

$$\int_{x_0}^{x_1} f(x)dx = (x_1 - x_0) \frac{f(x_0) + f(x_1)}{2} + E$$

You should note the order of accuracy as $O(h^2)$, $O(h^4)$ and $O(h^4)$ for the Trapezoidal, Simpson's and Simpson's 3/8 methods.

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12}f''(c)$$

Composite Rules are used in order to apply the integral formula over an interval $[a, b]$ which has been subdivided ($a = x_0 < x_1 < x_2 < \dots < x_n = b$), so we return to a more general quadrature formula

$$\begin{aligned} \int_a^b f(x)dx &\approx Q_h[f] = \sum_{j=0}^{n-1} \frac{h}{2}(f_j + f_{j+1}) \\ &= \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \dots + \frac{h}{2}(f_{n-1} + f_n) \\ &= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \dots + 2f_{n-1} + f_n) \\ &= \frac{h}{2} \left(f_0 + f_n + 2 \sum_{j=1}^{n-1} f_j \right) \end{aligned}$$

Improving accuracy of the method taking the composite rule for a step size of $2h$ instead of the original step size of size h :

$$\begin{aligned}
 \int_a^b f(x)dx &\approx Q_{2h}[f] = \sum_{j=0}^{n/2-1} \frac{2h}{2}(f_{2j} + f_{2j+2}) \\
 &= h(f_0 + f_2) + h(f_2 + f_4) + \dots + h(f_{n-2} + f_n) \\
 &= h(f_0 + 2f_2 + 2f_4 + \dots + 2f_{n-2} + f_n) \\
 &= h \left(f_0 + f_n + 2 \sum_{j=1}^{n/2-1} f_{2j} \right)
 \end{aligned}$$

Comparing this with $Q_h[F]$ we see that

$$Q_h[f] = \frac{1}{2}Q_{2h}[f] + h(f_1 + f_3 + \dots + f_{n-1})$$

This shows that we can improve accuracy by halving the step size h and this may be applied in order to obtain a desired accuracy.

Next week we'll cover the MATLAB built in functions. Here we implement the Trapezoidal method using the formula:

```
% Integrate the function  $x^2$  over a domain  
%  $x = [1,5]$  given a step size of  $h = .2$   
h = 0.2;
```

```
% Calculate the number of points needed  
n = (5-1)/h;  
x = (1+h:h:5);  
f0 = 12;  
f(1:n) = x(1:n).^2;  
Trap = (h/2)*(f0+f(n)+2*sum(f(1:n-1)))
```

```
% Compare the result with the actual integral  
(53-13)/3
```