Improving Quadrature Formulas

Up to this point we have been constructing quadrature formulas by interpolating integrands at a set of evenly spaced sample points and using the integrals of the interpolating polynomials to estimate the integral of the original integrand. A degree of freedom that we did not take advantage of in that process is the freedom to move the interpolation points around in the interval. What happens when we allow the interpolation points to float and try to optimize our results by selecting the best set of interpolating points?

One thing that is not immediately clear is whether or not the choice of optimal interpolation points can be made independent of the integrand. It turns out that they can, which is the basis for a general method called Gaussian Quadrature.

Another thing we will need is a method to determine how good a set of quadrature points is. One useful measure is the following:

Definition A quadrature formula

$$\int_a^b f(x)\,\mathrm{d}\,x \approx \sum_{j=1}^{k} c_j\, f(x_j)$$

is said to be *exact to degree n* if it yields exact equality when $f(x)$ is any polynomial of degree n or less.

Orthogonal Polynomials

The key to the Gaussian Quadrature is a special set of polynomials called *orthogonal polynomials*. A set $p_1(x)$, $p_2(x)$, …, $p_n(x)$ of polynomials is orthogonal on an interval $[a,b]$ if

$$\int_a^b p_j(x)\, p_k(x)\,\mathrm{d}\,x = 0$$

for all $j \neq k$. Changing the interval $[a,b]$ will change the polynomials.

Another important characteristic of orthogonal polynomials is that if $p_n(x)$ is an orthogonal polynomial of degree n and $p(x)$ is any polynomial of degree less than n then

$$\int_a^b p(x)\, p_n(x)\,\mathrm{d}\,x = 0$$

One commonly used set of orthogonal polynomials are the Legendre polynomials, which are orthogonal on the interval [-1,1]. Another useful characteristic of these polynomials is that all of their roots are real and are all located in the interval [-1,1].

Gaussian Quadrature

The Gaussian Quadrature method uses the roots x_1, x_2, …, x_n of the n^{th} degree Legendre polynomial $P_n(x)$ on [-1,1] as interpolation points to produce an improved quadrature formula. The following theorem shows why this is a good choice.

Theorem If x_1, x_2, …, x_n are the roots of the n^{th} degree Legendre polynomial $P_n(x)$, $L_{n,k}(x)$ is the k^{th} Lagrange basis function formed from these roots, and

$$c_k = \int_{-1}^{1} L_{n,k}(x)\,\mathrm{d}\,x$$

then for any polynomial $P(x)$ of degree less than 2 n we have

$$\int_{-1}^{1} P(x)\,\mathrm{d}\,x = \sum_{k=1}^{n} c_k\,P(x_k)$$

Proof First, note that if $P(x)$ is any polynomial of degree n-1 or less we can interpolate the points $(x_1, P(x_1))$, $(x_2, P(x_2))$, … $(x_n, P(x_n))$ and get an exact equality:

$$P(x) = \sum_{k=1}^{n} P(x_k)\,L_{n,k}(x)$$

Integrating this equality gives

$$\int_{-1}^{1} P(x)\,\mathrm{d}\,x = \int_{-1}^{1} \sum_{k=1}^{n} P(x_k)\,L_{n,k}(x)\,\mathrm{d}\,x = \sum_{k=1}^{n} P(x_k) \int_{-1}^{1} L_{n,k}(x)\,\mathrm{d}\,x = \sum_{k=1}^{n} c_k\,P(x_k)$$

Since the Legendre polynomials are orthogonal on the interval [-1,1] we can go beyond this. Let $P(x)$ be any polynomial of degree less than 2 n and let $P_n(x)$ be the n^{th} Legendre polynomial. We form

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

where $Q(x)$ and $R(x)$ are the polynomial quotient and remainder that result when we divide $P_n(x)$ into $P(x)$. Note that since $P(x)$ has degree less than 2 n and $P_n(x)$ has degree n, both $Q(x)$ and $R(x)$ will have degree less than n.

Now note that

$$P(x_k) = Q(x_k)\,P_n(x_k) + R(x_k) = Q(x_k)\,0 + R(x_k) = R(x_k)$$

since the points x_k were chosen to be roots of $P_n(x)$. Consider what happens when we integrate $P(x)$:

$$\int_{-1}^{1} P(x)\,\mathrm{d}\,x = \int_{-1}^{1} Q(x)\,P_n(x) + R(x)\,\mathrm{d}\,x = \int_{-1}^{1} Q(x)\,P_n(x)\,\mathrm{d}\,x + \int_{-1}^{1} R(x)\,\mathrm{d}\,x$$

Since $P_n(x)$ is an orthogonal polynomial of degree n and $Q(x)$ has degree less than n we have

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

and

$$\int_{-1}^{1} P(x)\,\mathrm{d}\,x = \int_{-1}^{1} R(x)\,\mathrm{d}\,x = \sum_{k=1}^{n} c_k\,R(x_k) = \sum_{k=1}^{n} c_k\,P(x_k)$$

since $R(x)$ has degree less than n.

An important thing to note about the quadrature formula we have just developed is that the coefficients c_k do not depend on $P(x)$:

$$c_k = \int_{-1}^{1} L_{n,k}(x)\, \mathrm{d}\, x$$

This means that we can pre-compute and tabulate the roots x_1, x_2, …, x_n and coefficients c_k and reuse those for each new integrand we have to deal with.

Integrating on [a,b]

The one remaining limitation of the quadrature formula we developed above is that it requires us to integrate on the interval [-1,1]. If we have to integrate on an interval [a,b] instead, we have to make a slight adjustment. The trick we need is to do a change of variables that transforms the interval [a,b] into [-1,1]. The simplest such change of variables is

$$x = \frac{1}{2}\left(\left(b - a\right) t + a + b\right)$$

To use this we do

$$\int_{-1}^{1} f(x)\, \mathrm{d}\, x = \frac{b - a}{2} \int_{-1}^{1} f\left(\frac{(b\text{-}a)\, t + a + b}{2}\right) \mathrm{d}\, t$$

The latter integral can be computed by the method above.