Day 11: Adaptive Integration and Gaussian Quadrature

Jeff Parker

November 10th 2012

1 Adaptive Integration

Things to look for:

a) How does the code keep track of the sub intervals?

b) How does the code measure the errors?

c) How does it dole out permission to err?

d) Two computations are made for each interval. What is done with the results?

```
% Tim Sauer
function sum = adapquad(f,a0,b0,tol0)
sum=0; n=1; a(1)=a0; b(1)=b0; tol(1)=tol0; app(1)=trap(f,a,b);
while n > 0            % n is current position at end of the list
    c = (a(n)+b(n))/2; oldapp=app(n);
    app(n)=trap(f,a(n),c);app(n+1) = trap(f,c,b(n));
    if abs(oldapp-(app(n)+app(n+1))) < 3*tol(n)
        sum = sum + app(n) + app(n+1); % success
        n=n-1;                         % done with interval
    else                               % divide into two intervals
        b(n+1)=b(n); b(n)=c;           % set up new intervals
        a(n+1)=c;
        tol(n)=tol(n)/2; tol(n+1) = tol(n);
        n=n+1;                         % go to end of list, repeat
    end
end

function s=trap(f,a,b)
s = (f(a)+f(b))*(b-a)/2;
```

Compare to the version below: what improvements have been made?

```
% Cleve Moler
% Recursive call
[Q,k] = quadtxstep(F, a, b, tol, fa, fc, fb, varargin{:});
fcount = k + 3;
% ----------------------------------------------------------
function [Q,fcount] = quadtxstep(F,a,b,tol,fa,fc,fb,varargin)
h = b - a;
c = (a + b)/2;
fd = F((a+c)/2,varargin{:});
fe = F((c+b)/2,varargin{:});
Q1 = h/6 * (fa + 4*fc + fb);
Q2 = h/12 * (fa + 4*fd + 2*fc + 4*fe + fb);
if abs(Q2 - Q1) <= tol
   Q  = Q2 + (Q2 - Q1)/15;
   fcount = 2;
else
   [Qa,ka] = quadtxstep(F, a, c, tol, fa, fd, fc, varargin{:});
   [Qb,kb] = quadtxstep(F, c, b, tol, fc, fe, fb, varargin{:});
   Q  = Qa + Qb;
   fcount = ka + kb + 2;
end
```

2 Gaussian Quadrature

The goal is to find a series of $(x_0, x_1, x_2, \ldots, x_n)$ and weights $(c_0, c_1, c_2, \ldots c_n)$ such that

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=0}^{i=n} c_i f(x_i)$$

Further, we want the results to be exact for polynomials of degree less than $2n-1$.

The two point method uses the points $\pm\frac{1}{\sqrt{3}}$ and the weights $(1,1)$ so that

$$\int_{-1}^{1} f(x)dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

We will derive the points and weights by using the method of undetermined coefficients. But to really understand the method, we need to understand Orthogonal Polynomials.

3 Orthogonal Polynomials

To see if two polynomials are orthogonal, we define an inner product on the set of functions. To start, we will restrict ourselves to the interval $[-1, 1]$.

The inner product of two vectors is the sum of the product of each pair of terms from the two vectors. We do something equivalent for functions: we define

$$< f, g > \stackrel{\text{def}}{=} \int_{-1}^{1} g(x) f(x) dx$$

We will show how these are useful in a later section. But first we will build an important orthogonal basis. the Legendre polynomials. We define

$$p_0(x) = 1 \qquad\qquad p_1(x) = x \tag{1}$$

A quick check shows that they are orthogonal: their inner product is zero.

$$< p_0, p_1 >= \int_{-1}^{1} p_0(x) p_1(x) dx = \int_{-1}^{1} x dx = \left.\frac{x^2}{2}\right|_{-1}^{1} = 0$$

We might try $f(x) = x^2$ as our quadratic basis function. It passes one test:

$$< p_1, f >= \int_{-1}^{1} p_1(x) f(x) dx = \int_{-1}^{1} x^3 dx = \left.\frac{x^4}{4}\right|_{-1}^{1} = 0$$

However, $f(x)$ is not orthogonal to $p_0(x)$, since

$$< p_0, f >= \int_{-1}^{1} p_0(x) f(x) dx = \int_{-1}^{1} x^2 dx = \left.\frac{x^3}{3}\right|_{-1}^{1} = \frac{2}{3}$$

We can proceed using the method of undetermined coefficients, setting $f(x) = x^2 + ax + b$ and looking for a and b. But it is simpler to apply the GramSchmidt process to make $f(x) = x^2$ orthogonal to $p_0(x)$ and $p_1(x)$.

$$p_2(x) = f(x) - p_0 \frac{< p_0, f(x) >}{< p_0, p_0 >} - p_1 \frac{< p_1, f(x) >}{< p_1, p_1 >}$$

$$p_2(x) = x^2 - \frac{\int_{-1}^{1} x^2 dx}{\int_{-1}^{1} dx} - x \frac{\int_{-1}^{1} x^3 dx}{\int_{-1}^{1} x^2 dx} = x^2 - \frac{\frac{2}{3}}{2} - \frac{0}{\frac{2}{3}} x = x^2 - \frac{1}{3}$$

Note that the zeros of $p_2(x)$ are $\pm\frac{1}{\sqrt{3}}$, the abscissa for our two point method.

Let's compute $p_3(x)$, starting with the cubic $f(x) = x^3$. By convention, all our basis vectors will be monic. We could insist that they be unit vectors instead.

$$p_3(x) = f(x) - p_0\frac{< p_0, f(x) >}{< p_0, p_0 >} - p_1\frac{< p_1, f(x) >}{< p_1, p_1 >} - p_2\frac{< p_2, f(x) >}{< p_2, p_2 >}p_2$$

As a short cut to evaluating these, note that the integral from -1 to 1 of any odd function is zero. This lets us skip the first and last inner products, leaving us with

$$p_3(x) = f(x) - p_1\frac{< p_1, f(x) >}{< p_1, p_1 >} = x^3 - x\frac{\int_{-1}^{1} x^4 dx}{\int_{-1}^{1} x^2 dx} = x^3 - x\frac{2/5}{2/3} = x^3 - \frac{3}{5}x$$

The zeros of $p_3(x)$ are the abscissa for the three point Gaussian Quadrature. We haven't seen why this should be, and other than the method of undetermined coefficients, we don't yet have a way to find the weights.

4 Example: Derive Three Point Rule

Let's see if we can derive the three point rule for Gaussian Quadrature on the interval $[-1, 1]$ using the method of Undetermined Coefficients. We will not use $p_3(x)$ to derive them.

We are looking for three abscissa, (x_0, x_1, x_2) and three weights (c_0, c_1, c_2) such that

$$\int_{-1}^{1} f(x)dx \approx c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2)$$

Further, we want the results to be exact for polynomials of degree less than 6.

By symmetry, we will assume that $x_1 = 0$ and $x_0 = -x_2$

If we let $f(x) = 1$ then $f(x_0) = f(x_1) = f(x_2) = 1$ and we find

$$2 = \int_{-1}^{1} dx = c_0 + c_1 + c_2$$

Next we set $f(x) = x$ and find that

$$0 = \int_{-1}^{1} x dx = c_0 x_0 + c_1 0 + c_2 x_2 = c_0 x_0 + c_2 x_2$$

If $x_0 = -x_2$ this implies that $c_0 = c_2$ as well.

From $f(x) = x^2$ we derive

$$\frac{2}{3} = \int_{-1}^{1} x^2 dx = c_0 x_0^2 + c_2 x_2^2$$

which tells us that $c_0 x_0^2 = \frac{1}{3}$

From $f(x) = x^3$ we derive

$$0 = \int_{-1}^{1} x^3 dx = c_0 x_0^3 + c_2 x_2^3$$

This tells us nothing new, since we assume $x_0 = -x_2$. From $f(x) = x^4$ we learn that

$$\frac{2}{5} = \int_{-1}^{1} x^4 dx = c_0 x_0^4 + c_2 x_2^4$$

Since $c_0 x_0^4 = \frac{1}{5}$ and $c_0 x_0^2 = \frac{1}{3}$, we can divide and see that $x_0^2 = \frac{3}{5}$ or $x_0 = \frac{\sqrt{3}}{\sqrt{5}} = \frac{\sqrt{15}}{5}$.

Substituting back, we use $c_0 x_0^2 = \frac{1}{3}$ and replace x_0^2 with $\frac{3}{5}$ to see $c_0 = \frac{5}{9}$. Since $c_0 = c_2$ and $c_0 + c_1 + c_2 = 2$, we see that $c_1 = 2 - \frac{10}{9} = \frac{8}{9}$.

Our abscissa are $(x_0, x_1, x_2) = (-\frac{\sqrt{15}}{5}, 0, \frac{\sqrt{15}}{5})$ and our weights are $(c_0, c_1, c_2) = (\frac{5}{9}, \frac{8}{9}, \frac{5}{9})$

Note that the abscissa are the roots of $p_3(x) = x^3 - \frac{3}{5}x$, the third Legendre Polynomial.

5 Importance of Orthogonal polynomials

The goal of Gaussian integration was to provide a better way to approximate the integrals of functions. Let's run through an example, using three point integration. Assume we are trying to integrate $P(x) = x^5$ with three points.

We use synthetic division to express $P(x)$ in terms of $p_3(x)$.

$$x^5 = (x^3 - \frac{3}{5}x)(x^2 + \frac{3}{5}) + \frac{9}{25}x$$

We will name these parts:

$$P(x) = p_3(x)S(x) + R(x)$$

We then integrate both sides

$$\int_{-1}^{1} x^5 dx = \int_{-1}^{1} (x^3 - \frac{3}{5}x)(x^2 + \frac{3}{5}) dx + \int_{-1}^{1} \frac{9}{25} x dx$$

It isn't hard to believe that we can integrate $R(x)$ using it's values at three points, but we haven't been given it's values there: we only have the value of $P(x)$ at the three points.

Turn to the integral of $p_3(x)S(x)$. Since $p_3(x)$ is orthogonal to polynomials of degree less than 3, such as $S(x) = x^2 + \frac{3}{5}$, that integral is zero.

As far as evaluating the function $R(x)$ at the abscissa x_i, note that these points were chosen to be the zeros of $p_3(x)$, so that for $x_i \in \{0, \pm\sqrt{\frac{3}{5}}\}$,

$P(x_i) = p_3(x_i)S(x_i) + R(x_i) = 0 \times S(x_i) + R(x_i)$

Thus $P(x_i) = R(x_i)$ for each point.

One simpler example: we use $p_2(x) = x^2 - \frac{1}{3}$ and the two point method to evaluate an arbitrary cubic $P(x) = x^3 - 4x + 1$

$$P(x) = x^3 - 4x + 1 = (x^2 - \frac{1}{3})(x) + (1 - \frac{11}{3}x)$$

$$P(x) = p_2(x)S(x) + R(x)$$

$$\int_{-1}^{1} x^3 - 4x + 1 = \int_{-1}^{1} (x^2 - \frac{1}{3})(x)dx + \int_{-1}^{1} (1 - \frac{11}{3}x)dx$$

Again, the integral $\int_{-1}^{1}(x^2 - \frac{1}{3})(x)dx$ vanishes, as $p_2(x)$ is orthogonal to linear polynomials, and we can evaluate the integral of the linear function $R(x)$ at two points. We know the value of $R(x)$ there, as we will pick points where $p_2(x)$ vanishes, so $R(x_i) = P(x_i)$.

6 Theorem 5.6

The Gaussian Quadrature Method using the degree n Legendre polynomial on $[-1, 1]$, has degree of precision $2n - 1$.

Proof: Let $P(x)$ be a polynomial of degree $2n - 1$ or less. Using polynomial division to express this as

$$P(x) = p_n(x)S(x) + R(x)$$

Note that $S(x)$ and $R(x)$ are polynomials of degree $n - 1$ or less.

$$\int_{-1}^{1} P(x) = \int_{-1}^{1} p_n(x)S(x)dx + \int_{-1}^{1} R(x)dx$$

As in our examples, the integral of $p_n(x)S(x)$ vanishes, as p_n is orthogonal to polynomials of degree less than $n - 1$. Thus we have the identity

$$\int_{-1}^{1} P(x) = \int_{-1}^{1} R(x)dx$$

To integrate $P(x)$, we need only integrate $R(x)$. We could do so if we could evaluate $R(x)$ at n points. If we pick the points to be the zeros of $p_n(x)$, we can evaluate $R(x)$ by evaluating $P(x)$.