Gaussian Quadrature

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Introduction

Gaussian quadrature is an amazing technique for numerical integration. Generally when interpolating polynomials one needs \( n + 1 \) points to interpolate an \( n^{th} \) degree polynomial. The same could be expected for numerical integration. However Gaussian quadrature integrates polynomials of degree \( 2n + 1 \) exactly with \( n + 1 \) points. This is a very powerful technique.

Quadratures

A numerical quadrature is a scheme, which is used to approximate the integral of a given function over a finite interval. The following is known as the Newton-Cotes formula, the right hand side is an approximation of the the integral on the left hand side, where the \( a_i \) are coefficients, and \( x_i \) are roots:

\[
\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i), \quad x_i \in [a, b]. \tag{1}
\]

Different formulas give different \( a_i \), the Newton-Cotes formulas chooses the \( x_i \) evenly. Generally this is a straight-forward approach and easily understandable and implementable. On large intervals, the Newton-Cotes formulas have an error of order \( h^k \) where \( h \) is step size of \( x_i \) and \( k \) is greater than one and depends on the method used. Another quadrature is Gaussian quadrature, which chooses \( x_i \) and \( a_i \) such that the error is minimized. This choice of \( x_i \) is made by finding the roots of an \( n^{th} \)-order Legendre polynomial \( P_n(x) \).

The family of Legendre polynomials are a collection of polynomials, \( \{P_0(x), P_1(x), \ldots, P_n(x), \ldots \} \), where the polynomials are monic and orthogonal to each other with respect to \( \omega(x) = 1 \). Orthogonality in this context is with respect to the \( L_2 \) inner product, i.e.,

\[
\int_{-1}^{1} P_n(x)P_m(x)dx = 0
\]

except when \( n = m \).

Gaussian Quadrature chooses \( x_i \), and \( c_i \) for \( i = 1, 2, \ldots, n \), such that:

\[
\int_{-1}^{1} P(x)dx \approx \sum_{i=1}^{n} c_i P(x_i), \quad x_i \in [-1, 1]. \tag{2}
\]

The integral on the left hand side is equal to the sum on the right hand side for any polynomial, \( P(x) \), of degree strictly less than \( 2n \).\(^\text{1}\)

\(^\text{1}\)Burden-Faires Numerical Analysis 8th ed., pg 223
How do we find the polynomials such that the above equation holds. For a polynomial of degree 0 we use the easiest such polynomial, $P_0(x) = 1$. Likewise for a polynomial of degree 1 we use $P_1(x) = x$. These polynomials are orthogonal and monic, however for polynomials where the degree is greater than two this will not work so conveniently, since we want the polynomials to be monic and orthogonal. This is where Gram-Schmidt orthogonalization comes in handy. We can use Gram-Scmidt to generalize the process for polynomials of degree $n > 2$, which constructs an orthonormal basis of functions. The Legendre polynomials, $P_0(x), P_1(x), \ldots$, are one such set of linearly independent functions. The points needed to give exact results (for a polynomial of degree less than $2n - 1$) for equation (2) are the roots of an $n^\text{th}$ degree Legendre polynomial. Likewise the weights, $c_i$, necessary for the right hand side of equation (2) come from the coefficients of the Legendre polynomials.

Formulation

The first step towards generating the roots, $x_i$, and weights, $c_i$, for Gaussian Quadrature is to construct the corresponding polynomials. By applying Gram-Schmidt orthogonalization to the polynomials $1, x^2, x^3, \ldots$, on the interval $[-1, 1]$ we construct the Legendre polynomials, which we can then use to find the roots and the coefficients. Gram-Schmidt orthogonalization uses the fact that the $L_2$ inner product of two different degree polynomials will be zero, but the $L_2$ inner product of two polynomials with the same degree will be one. Given this concept of the Gram-Schmidt orthogonalization, the actual calculation is given by a three term recursion formula, i.e., the $i^\text{th}$ polynomial (denoted $\phi_i$) may be written in terms of the $(i - 1)^\text{th}$ and the $(i - 2)^\text{th}$ polynomials.

$$
\phi_i(x) = (x - B_i)\phi_{i-1}(x) - D_i\phi_{i-2}(x) \tag{3}
$$

where $B_i = \frac{\int_{-1}^{1} x|\phi_{i-1}(x)|^2dx}{\int_{-1}^{1}|\phi_{i-1}(x)|^2dx}$ and $D_i = \frac{\int_{-1}^{1} x|\phi_{i-1}(x)\phi_{i-2}(x)|dx}{\int_{-1}^{1}|\phi_{i-2}(x)|^2dx}$

This formula may look different than the Gram-Schmidt formula we are familiar with for vectors. But it is not, for vectors we have:

$$
u_i = v_i - \sum_{l=1}^{i-1} \frac{<v_i, u_l>}{<u_l, u_l>} u_l \tag{4}
$$

where $<v_i, u_l>$ denotes the inner product between $v_i$ and $u_l$. In order to see that the idea is the same, think of $x\phi_i$ as the vector we
are projecting, let’s call it $v_i$. Then we have
\[
u_i = v_i - \frac{\langle v_i, v_{i-1} \rangle}{\langle v_{i-1}, v_{i-1} \rangle} v_{i-1} - \frac{\langle v_i, v_{i-2} \rangle}{\langle v_{i-2}, v_{i-2} \rangle} v_{i-2}
\]
which is our familiar Gram-Schmidt orthogonalization and is the same as (3) if we note that $u_i = \phi_i$. Additionally (3) is only a three term recursion, because if we carry out more terms all of the them will be zero since two different degree polynomials are orthogonal. Thus using Gram-Schmidt orthogonalization we build a family of orthogonal, monic polynomials. The next step in Gaussian quadrature is to then compute the roots, $x_i$, of these polynomials. This can be done relatively easy using Newton’s Method. Once the roots have been calculated the weights $c_i$ are found using the roots and Lagrange polynomials. We then have a quadrature that is exact for polynomials of degree $2n + 1$.

Another interesting linear algebra tidbit regarding Legendre polynomials is the fact that the Legendre differential equation is:
\[
\frac{d}{dx}[(1-x^2)\frac{d}{dx}P(x)] = -\lambda P(x)
\]
which is just an eigenvalue problem. It turns out that the Legendre polynomials are the eigenfunctions of this particular operator.

**Example**

In this section we will demonstrate an example in which we find the Legendre polynomials up to degree 3, then use those to calculate the integral of the polynomial of degree 5 exactly, e.g., $\int_{-1}^{1} 5x^3 - 7x^2 + x + 4 dx$ will be calculated exactly using a polynomial of degree 3.

First we start with the easiest polynomial, $P_0(x) = 1$. We apply G-S (Gram-Schmidt orthogonalization). $P_1(x) = x - \frac{\langle x, 1 \rangle}{\langle 1, 1 \rangle} = x - \frac{\int_{-1}^{1} x^2 dx}{\int_{-1}^{1} 1 dx}$, which we swiftly calculate to be, $P_1(x) = x$. Next is, $P_2(x)$, which is not so straightforward, but still not too bad, we’re just integrating polynomials, using (G-S) $P_2(x) = x^2 - \frac{\langle x^2, x \rangle}{\langle x, x \rangle} x - \frac{\langle x^2, 1 \rangle}{\langle 1, 1 \rangle} = x^2 - \frac{\int_{-1}^{1} x^2 dx}{\int_{-1}^{1} x^2 dx} x - \frac{\int_{-1}^{1} x^2 dx}{\int_{-1}^{1} 1 dx}$. Computing the necessary integrals we arrive at $P_2(x) = x^2 - 1/3$. Following the same blueprint we arrive at $P_3(x) = x^3 - 3/5 x$.

Now that we have our family of polynomials we set about finding the roots. Using Newton’s Method, $x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$ makes short work out of an otherwise difficult task. I used Matlab, but
Maple and Mathematica also have root finders. The roots and the respective coefficients are:

<table>
<thead>
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<th>n</th>
<th>roots</th>
<th>coefficients</th>
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</thead>
<tbody>
<tr>
<td>2</td>
<td>0.5773502</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>-0.5773502</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>0.7745966</td>
<td>0.5555556</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0.8888889</td>
</tr>
<tr>
<td></td>
<td>-0.7745966</td>
<td>0.5555556</td>
</tr>
</tbody>
</table>

We can now use these values to calculate the value of the integral:

\[
\int_{-1}^{1} 5x^5 - 7x^3 + x + 4\,dx = \quad (7)
\]

\[
\begin{align*}
&\frac{5}{5}(0.7745966)^5 - 7(0.7745966)^3 + 0.7745966 + 4 + 0.8 \times 4 + 8 \quad (8) \\
&\frac{5}{5}(-0.7745966)^5 - 7(-0.7745966)^3 - 0.7745966 + 4 \quad (9)
\end{align*}
\]

which my computer calculated to be 8.000000. Integrating the left hand side, we arrive at

\[
\frac{5}{6}x^6 - \frac{7}{4}x^4 + \frac{x^2}{2} + 4x \bigg|_{-1}^{1} = \frac{43}{12} - \frac{-53}{12} = 8.
\]

How cool is that? We plugged in the roots and weights from a third degree polynomial and got an exact result of a fifth degree polynomial. In other words with a third degree polynomial we were able to calculate the integral of a fifth degree polynomial exactly.

So where would you use this? Taylor series comes to mind, suppose you have a nasty integral, which you can not evaluate by hand, you could approximate it with a Taylor series and then use Gaussian Quadrature and get a respectable answer.