Note on Numerical Integration: Gaussian Quadrature

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1 Motivation

Remember how the trapezoid rule and Simpson's rule look like. With N points, trapezoid rule and the Simpson's rule approximate the integral by the following formula (let $h = \frac{(\overline{x}-\underline{x})}{(N-1)}$)

$$\int_{\underline{x}}^{\overline{x}} f(x)dx \simeq \left(\frac{h}{2}f(x_1) + hf(x_2) + hf(x_3) + hf(x_4) + ... + hf(x_{N-1}) + \frac{h}{2}f(x_N)\right)$$

$$\int_{\underline{x}}^{\overline{x}} f(x)dx \simeq \left(\frac{h}{3}f(x_1) + \frac{4h}{3}f(x_2) + \frac{2h}{3}f(x_3) + \frac{4h}{3}f(x_4) + ... + \frac{4h}{3}f(x_{N-1}) + \frac{h}{3}f(x_N)\right)$$

Notice that both formula can be rewritten as:

$$\int_{\underline{x}}^{\overline{x}} f(x)dx \simeq \sum_{i=1}^{N} \omega_i f(x_i)$$

For some $\{\omega_i\}_{i=1}^N$.

In other words, both of the Newton-Coates quadrature formula approximate the integral with $2N$ parameters, which consists of N points and N weights to each point.

Newton-Coates quadratures set a simple rule for the choice of the grid points (set points so that the entire interval is separated into equally-distanced subintervals) and concentrate on the choice of the weights to each point. Actually, as we have seen with Romberg Integration, using equally-spaced grid points helps using higher order approximation or adaptive procedure easily.

Instead, Gaussian quadrature is trying to choose all of $2N$ parameters, such that the approximation of the integral is "good" using certain criteria. The question is "how do we define the goodness?"

Suppose we use polynomial approximation of $f(x)$ function. Since we have $2N$ parameters to pinned down, if we use a polynomial of degree $2N-1$, all the parameters can be exactly pinned down.

In other words, if the true $f(x)$ function is a polynomial order less or equal to $2N-1$, the integral using polynomial approximation will give exact value of the integral. Formally, if $f(x)$ is a polynomial of order less than or equal to $2N-1$, we can find $\{x_i\}_{i=1}^N$ and $\{\omega_i\}_{i=1}^N$ such that the following always holds:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} \omega_i f(x_i)$$

This is the measure of "goodness" used for Gaussian quadrature. If a Gaussian quadrature method is used, an integral of $f(x)$ over some interval (let's use $[-1,1]$ without loss of generality), can be exactly obtained if $f(x)$ is a polynomial of order less than or equal to $2N-1$. If the order of $f(x)$ is higher, the Gaussian quadrature gives an approximation of the true integral.

2 Gauss-Legendre Quadrature

Let's start by stating a theorem.

Theorem 1 (Gauss-Legendre Quadrature)
Suppose $\{x_i\}_{i=1}^N$ are the roots of order N Legendre polynomial $P_N(x)$. Define $\{\omega_i\}_{i=1}^N$ such that:

$$\omega_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j} dx$$

If $f(x)$ is a polynomial of degree equal to or less than $2N-1$, then the following equation holds:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} \omega_i f(x_i)$$

First of all, the following result is helpful in proving the theorem:

Proposition 1 (Lagrange Interpolation Formula)
Suppose we want to approximate a function $f(x)$ by a polynomial $\tilde{f}(x)$. Suppose we have $\{x_i\}_{i=1}^N$ and $\{f(x_i)\}_{i=1}^N$. (This type of data is called Lagrange data). Since we have N conditions to identify $\tilde{f}(x)$, we can construct $\tilde{f}(x)$ which is identical to $f(x)$ if $f(x)$ is a polynomial of order equal to or less than $N-1$. In particular, we can construct such $\tilde{f}(x)$ as follows:

$$\tilde{f}(x) = \sum_{i=1}^{N} \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j} f(x_i)$$

Also remember that Legendre polynomial is a family of orthogonal polynomials, defined over $[-1, 1]$, with a trivial weighting function $w(x) = 1$. Now let's prove.

Proof 1 (Gauss-Legendre Quadrature)

1. *In case $f(x)$ is a polynomial of order equal or less than $N-1$. Construct $\{x_i\}_{i=1}^N$ such that they are the N roots of $P_N(x)$. Use the Lagrange interpolation formula to construct $\tilde{f}(x)$. Then:*

$$\begin{aligned}
\int_{-1}^{1} f(x)dx &= \int_{-1}^{1} \left(\sum_{i=1}^{N} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j} f(x_i) \right) dx \\
&= \sum_{i=1}^{N} \left(\int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j} f(x_i) \right) dx \\
&= \sum_{i=1}^{N} \omega_i f(x_i)
\end{aligned}$$

   This implies that if $\{\omega_i\}_{i=1}^N$ are chosen in a way specified in the theorem, the integral of $f(x)$ can be exactly obtained by the formula in the theorem.

2. *Now, consider the case when $f(x)$ is a polynomial of order higher than $N-1$ but equal to or less than $2N-1$. First, if we divide $f(x)$ by $P_N(x)$ (which is a polynomial of order equal to or less than $f(x)$), we can obtain the following:*

$$f(x) = P_N(x)Q(x) + R(x)$$

where both $Q(x)$ and $R(x)$ are polynomials f order equal to or less than $N-1$. Using this:

$$\begin{aligned}\int_{-1}^{1} f(x)dx &= \int_{-1}^{1} P_N(x)Q(x) + R(x)dx \\ &= \int_{-1}^{1} P_N(x)Q(x)dx + \int_{-1}^{1} R(x)dx\end{aligned}$$

Remember that $P_N(x)$ is a Legendre orthogonal, whose weighting function is $w(x) = 1$. In addition, $Q(x)$ can be represented by linear combination of the Legendre polynomials up to order $N-1$. Since orthogonality implies that the product of each of such Legendre polynomials and $P_N(x)$ integrates to zero, we get the following:

$$\int_{-1}^{1} P_N(x)Q(x)dx = 0$$

On the other hand, remember that $R(x)$ is a polynomial of order equal to or less than $N-1$. Using the previous result (case 1), we know that the integral of $R(x)$ can be exactly represented, using N roots of $P_N(x)$ as $\{x_i\}_{i=1}^N$, as follows:

$$\int_{-1}^{1} R(x)dx = \sum_{i=1}^{N} \omega_i R(x_i)$$

Next, remember how we obtain $Q(x)$ and $R(x)$. They satisfy:

$$f(x) = P_N(x)Q(x) + R(x)$$

Remember we choose $\{x_i\}_{i=1}^N$ such that they are the N roots of $P_N(x)$, therefore, for $i = 1, 2, ..., N$:

$$f(x_i) = P_N(x_i)Q(x_i) + R(x_i) = R(x_i)$$

Combining all we got above, we get:

$$\begin{aligned}
\int_{-1}^{1} f(x)dx &= \int_{-1}^{1} P_N(x)Q(x) + R(x)dx \\
&= \int_{-1}^{1} P_N(x)Q(x)dx + \int_{-1}^{1} R(x)dx \\
&= \int_{-1}^{1} R(x)dx \\
&= \sum_{i=1}^{N} \omega_i R(x_i) \\
&= \sum_{i=1}^{N} \omega_i f(x_i)
\end{aligned}$$

This completes the proof.

3 Change of Variables

So far, we have ignored the fact that we usually want to integrate $f(x)$ over $[\underline{x}, \overline{x}]$, not over $[-1, 1]$. We have been using $[-1, 1]$ because it's easy to relate to Legendre polynomials. However, as you can imagine, it's easy to convert the variables so that we can integrate $f(x)$ over $[\underline{x}, \overline{x}]$. Let's see how.

Denote z is a point on $[-1, 1]$ and x is a point on $[\underline{x}, \overline{x}]$. Consider a simple mapping from $[-1, 1]$ to $[\underline{x}, \overline{x}]$ as follows:

$$g_z(x) = z = \frac{2x - \underline{x} - \overline{x}}{\overline{x} - \underline{x}}$$

It's equivalent to:

$$g_x(z) = x = \frac{1}{2}[(\overline{x} - \underline{x})z + \underline{x} + \overline{x}]$$

Notice:

$$\frac{d\ g_x(z)}{dz} = \frac{\overline{x} - \underline{x}}{2}$$

Using this, Gauss-Legendre quadrature formula can be rewritten as follows:

$$\begin{aligned}
\int_{\underline{x}}^{\overline{x}} f(x)dx &= \int_{-1}^{1} f(g_x(z))\frac{d\ g_x(z)}{dz}\ dz \\
&= \int_{-1}^{1} f\left(\frac{(\overline{x} - \underline{x})z + \underline{x} + \overline{x}}{2}\right) \frac{\overline{x} - \underline{x}}{2}dz \\
&= \frac{\overline{x} - \underline{x}}{2} \sum_{i=1}^{N} \omega_i f(g_x(z_i))
\end{aligned}$$

where $\{z_i\}_{i=1}^N$ and $\{\omega_i\}_{i=1}^N$ are constructed in the same way as the theorem states.

Now let's summarize:

Algorithm 1 (Gauss-Legendre Quadrature)

1. *Suppose we want to approximate numerically:*

$$\int_{\underline{x}}^{\overline{x}} f(x)\ dx$$

2. *Choose N. It implies that Legendre polynomial of order $N-1$ is going to be used to approximate $f(x)$.*

3. *Compute N roots of order N Legendre polynomial $P_N(z)$. Denote them as $\{z_i\}_{i=1}^N$. Actually, you should be able to get the roots of Legendre polynomials from any books on numerical methods.*

4. *Construct $\{x_i\}_{i=1}^N$ using:*

$$x_i = \frac{(\overline{x} - \underline{x})z_i + \underline{x} + \overline{x}}{2}$$

5. *Obtain $\{\omega_i\}_{i=1}^N$ using:*

$$\omega_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{N} \frac{x - x_j}{x_i - x_j} dx$$

   Actually it's not easy compute ω_i but you can find the values in any books on numerical methods.

6. *The approximated integral can be computed by:*

$$\int_{\underline{x}}^{\overline{x}} f(x) dx \simeq \frac{\overline{x} - \underline{x}}{2} \sum_{i=1}^{N} \omega_i f(x_i)$$

   Remember that, if $f(x)$ is a polynomial of order equal to or less than $2N-1$, this formula gives the exact value of the integral.

4 Gauss-Chebyshev Quadrature

We studied Gauss-Legendre quadrature, because the weighting function associated with Legendre polynomials is a trivial one. But the method can be extended to any family of orthogonal polynomials.

Let's extend our result to Chebyshev polynomials:

Theorem 2 (Gauss-Chebyshev Quadrature)
Suppose $\{x_i\}_{i=1}^N$ *are the roots of order* N *Chebyshev polynomial* $P_N(x)$*. Define* $\{\omega_i\}_{i=1}^N$ *such that:*

$$\omega_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j} \frac{1}{\sqrt{1-x^2}} \; dx = \frac{\pi}{N}$$

If $f(x)$ *is a polynomial of degree equal to or less than* $2N-1$*, then the following equation holds:*

$$\int_{-1}^{1} f(x) \frac{1}{\sqrt{1-x^2}} \; dx = \sum_{i=1}^{N} \omega_i f(x_i)$$

A couple of comments below:

1. A great thing about Chebyshev is that the weights and grid points are really simple.

2. Weights are actually constant! Weights are:

$$\omega_i = \frac{\pi}{N}$$

3. Roots can be computed by the following formula:

$$x_i = -\cos\left(\frac{2i-1}{2N}\pi\right)$$

4. We can use the same trick to convert the domain from $[-1, 1]$ to $[\underline{x}, \overline{x}]$.

5. There is another problem. Chebyshev has nontrivial weighting function, which most of the times we do not want. But we can solve this problem by redefining the integrand by multiplying the inverse of the weighting function.

Taking into account the remarks above, the algorithm looks like the following:

Algorithm 2 (Generalized Gauss-Chebyshev Quadrature)

1. *Suppose we want to approximate numerically:*

$$\int_{\underline{x}}^{\overline{x}} f(x) \; dx$$

2. *Choose* N*. It implies that Chebyshev polynomial of order* $N-1$ *is going to be used to approximate* $f(x)$*.*

3. *Compute* N *roots of order* N *Chebyshev polynomial* $P_N(z)$*. Denote them as* $\{z_i\}_{i=1}^N$*. There is an easy formula to compute them:*

$$z_i = -\cos\left(\frac{2i-1}{2N}\pi\right)$$

4. *Construct* $\{x_i\}_{i=1}^N$ *using:*

$$x_i = \frac{(\overline{x} - \underline{x})z_i + \underline{x} + \overline{x}}{2}$$

5. *Set* $\{\omega_i\}_{i=1}^N$ *as follows:*

$$\omega_i = \frac{\pi}{N} \qquad \forall i$$

6. *The approximated integral can be computed by:*

$$\int_{\underline{x}}^{\overline{x}} f(x)dx \simeq \frac{\overline{x} - \underline{x}}{2} \sum_{i=1}^{N} \omega_i f(x_i)\sqrt{1 - z_i^2}$$

Remember that, if $f(x)$ *is a polynomial of order equal to or less than* $2N - 1$*, this formula gives the exact value of the integral.*

5 Gauss-Hermite Quadrature

Theorem 3 (Gauss-Hermite Quadrature)
Suppose $\{x_i\}_{i=1}^N$ *are the roots of order* N *Hermite polynomial* $P_N(x)$*. Define* $\{\omega_i\}_{i=1}^N$ *such that:*

$$\omega_i = \int_{-\infty}^{\infty} \prod_{\substack{j=1 \\ j \neq i}}^{N} \frac{x - x_j}{x_i - x_j} \; e^{-x^2} \; dx$$

If $f(x)$ *is a polynomial of degree equal to or less than* $2N - 1$*, then the following equation holds:*

$$\int_{-\infty}^{\infty} f(x) \; e^{-x^2} \; dx = \sum_{i=1}^{N} \omega_i f(x_i)$$

The shape of the weighting function associated with Hermite polynomials motivate the numerical integration using normal distribution as weighting function.
In particular, consider an expectation of $f(z)$ where z is distributed as $N(\mu, \sigma^2)$. What we want to compute is:

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(z) \; e^{-\left(\frac{z-\mu}{\sqrt{2}\sigma}\right)^2} \; dz$$

First of all, define x as:

$$x = \frac{z - \mu}{\sqrt{2}\sigma}$$

Equivalently:

$$z = \sqrt{2}\sigma x + \mu$$

Replace z with x in the integration, and we get:

$$\begin{aligned}(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(z)\ e^{-\left(\frac{z-\mu}{\sqrt{2}\sigma}\right)^2}\ dz &= (2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(\sqrt{2}\sigma x+\mu)\ e^{-x^2}\ \sqrt{2}\sigma\ dx \\ &= \sqrt{2}\sigma(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(\sqrt{2}\sigma x+\mu)\ e^{-x^2}\ dx \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(\sqrt{2}\sigma x+\mu)\ e^{-x^2}\ dx\end{aligned}$$

Using the theorem, we can obtain:

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(z)\ e^{-\left(\frac{z-\mu}{\sqrt{2}\sigma}\right)^2}\ dz = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{N} \omega_i f(\sqrt{2}\sigma x_i+\mu)$$

where $\{x_i\}_{i=1}^N$ and $\{\omega_i\}_{i=1}^N$ are described in the theorem.

Let's summarize:

Algorithm 3 (Gauss-Hermite Quadrature associated with Normal Distribution)

1. *Suppose we want to approximate numerically an expectation of $f(z)$, where z is distributed by $N(\mu,\sigma^2)$. In other words, we want to compute:*

   $$E_z f(z) = (2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(z)\ e^{-\left(\frac{z-\mu}{\sqrt{2}\sigma}\right)^2}\ dz$$

2. *Choose N. It implies that Hermite polynomial of order $N-1$ is going to be used to approximate $f(z)$.*

3. *Compute N roots of order N Hermite polynomial $P_N(x)$. Denote them as $\{x_i\}_{i=1}^N$. Since there is no simple formula for the roots, the easiest way is to find in a book on numerical methods.*

4. *Construct $\{z_i\}_{i=1}^N$ using:*

   $$z_i = \sqrt{2}\sigma x_i + \mu$$

5. *Set $\{\omega_i\}_{i=1}^N$ as follows:*

   $$\omega_i = \int_{-\infty}^{\infty} \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x-x_j}{x_i-x_j}\ e^{-x^2}\ dx$$

   Again, the simplest way to obtain $\{\omega_i\}_{i=1}^N$ is to find in a book.

6. *The approximated integral can be computed by:*

   $$E_z f(z) = (2\ pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(z)\ e^{-\left(\frac{z-\mu}{\sqrt{2}\sigma}\right)^2}\ dz = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{N} \omega_i f(z_i)$$

   Remember that, if $f(z)$ is a polynomial of order equal to or less than $2N-1$, this formula gives the exact value of the integral.

A comment below:

1. Good example of how to use the Gauss-Hermite quadrature is given in Judd (pp262-263). In the model the quadrature method is used to compute the expected value of an investor when the return of assets follow normal distributions.

6 Gauss-Laguerre Quadrature

I am going to state only the theorem. Judd (pp263-264) exhibits an example where Gauss-Laguerre quadrature is useful.

Theorem 4 (Gauss-Laguerre Quadrature)
Suppose $\{x_i\}_{i=1}^N$ are the roots of order N Laguerre polynomial $P_N(x)$. Define $\{\omega_i\}_{i=1}^N$ such that:

$$\omega_i = \int_0^\infty \prod_{\substack{j=1 \\ j\neq i}}^N \frac{x - x_j}{x_i - x_j} \; e^{-x} \; dx$$

If $f(x)$ is a polynomial of degree equal to or less than $2N-1$, then the following equation holds:

$$\int_0^\infty f(x) \; e^{-x} \; dx = \sum_{i=1}^N \omega_i f(x_i)$$