Gaussian Quadrature

• Recall our general quadrature formula

\[ \int_a^b f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i) \quad (1) \]

where the \( w_i \) are the \textbf{weights} and the \( x_i \) are the \textbf{knots}.

• Note that today we start with \( i = 1 \) instead of \( i = 0 \).

• If the knots are evenly spaced we have a \textbf{Newton-Cotes Formula}.

• In Gaussian Quadrature we pick both the weights and the knots so as to obtain exactness for polynomials of degree as high as possible.

• Moreover, we generalize the formula (1) to include the possibility of having a positive weight function \( w(x) > 0 \). Thus we consider the more general formula

\[ \int_a^b w(x)f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i) \quad (2) \]
We want this formula to be exact when \( f \) (and not the whole integrand \( w(x)f(x) \)) is a polynomial of degree as high as possible.

Note that

\[ w_i \neq w(x_i) \]

- One application of having a weight function is to accommodate improper integrals. For example, we could use
  - **Legendre**, ordinary integrals as before:
    \[
    I = \int_{-1}^{1} f(x)dx, \quad w(x) = 1, \quad [a, b] = [-1, 1]
    \]
  - **Chebychev**, the integrand is singular at the end points:
    \[
    I = \int_{-1}^{1} \frac{1}{\sqrt{1 - x^2}} f(x)dx, \quad w(x) = \frac{1}{\sqrt{1 - x^2}}, \quad [a, b] = [-1, 1]
    \]
  - **Laguerre**, the interval is semi-infinite:
    \[
    I = \int_{0}^{\infty} e^{-x} f(x)dx, \quad w(x) = e^{-x}, \quad [a, b] = [0, \infty)
    \]
  - **Hermite**, we are integrating over the whole real line:
    \[
    I = \int_{-\infty}^{\infty} e^{-x^2} f(x)dx, \quad w(x) = e^{-x^2}, \quad (a, b) = (-\infty, \infty)
    \]
Method of Undetermined Coefficients

- As we did for Simpson’s Rule, we can use the method of undetermined coefficients to obtain a system of equations for the knots and the weights.

However, that system is **nonlinear**!

- For example, consider the case $n = 2$, $[a, b] = [-1, 1]$ and $w(x) = 1$.

$$
\int_{-1}^{1} f(x) dx \approx w_1 f(x_1) + w_2 f(x_2)
$$

which is exact if $f$ is a polynomial of degree up to 3.

- We get the **nonlinear** $4 \times 4$ system:

\[
\begin{align*}
  f(x) &= 1 & \int_{-1}^{1} 1 \, dx &= 2 &= w_1 + w_2 \\
  f(x) &= x & \int_{-1}^{1} x \, dx &= 0 &= w_1 x_1 + w_2 x_2 \\
  f(x) &= x^2 & \int_{-1}^{1} x^2 \, dx &= 2/3 &= w_1 x_1^2 + w_2 x_2^2 \\
  f(x) &= x^3 & \int_{-1}^{1} x^3 \, dx &= 0 &= w_1 x_1^3 + w_2 x_2^3 
\end{align*}
\]

- In general, nonlinear systems can be very hard to solve.

- However, it is easy to check that the system
(3) has the solution

\[ w_1 = 1 \]
\[ w_2 = 1 \]
\[ x_1 = -\frac{\sqrt{3}}{3} \]
\[ x_2 = \frac{\sqrt{3}}{3} \]

- This is pretty remarkable!

- Carl Friedrich Gauss (1777-1855) managed to solve problems like (3) in great generality.

- How he did this is our next topic.

- So, again, we want to find weights \( w_1 \) and knots \( x_i, i = 1, \ldots, n \) such that the formula

\[
\int_a^b w(x)f(x)dx \approx \sum_{i=1}^n w_i f(x_i)
\]

is exact for polynomials \( f \) of degree as high as possible.

How high is possible?
• Let $p$ be a polynomial of degree $2n - 1$.

• The nonlinear system is linear in the coefficients $w_i$, so we need to break the polynomial $p$ into 2 pieces:

$$p(x) = Q_n(x)q(x) + r(x)$$

where $Q_n$ is a polynomial of degree $n$ that we will determine suitably.

• $q$ is the **quotient** and $r$ is the **remainder**. Both are polynomials of degree $n - 1$.

• Given $Q_n$ we can compute $q$ and $r$ by **long division**.

• Example:

$$n = 2$$

$$Q_2(x) = x^2 - \frac{1}{3}$$

$$p(x) = x^3 + 2x^2 + 3x + 4$$
How do we pick $Q_n$? We have

\[
I = \int_a^b w(x)p(x)dx \\
= \int_a^b w(x)(Q_n(x)q(x) + r(x))dx \\
= \int_a^b w(x)Q_n(x)q(x)dx + \int_a^b w(x)r(x)dx
\]

make this zero

So $Q_n$ must be a polynomial that is orthogonal to all lower degree polynomials with respect to the **inner product**:

\[
(f, g) = \int_a^b w(x)f(x)g(x)dx
\]

- We could compute these polynomials by the Gram-Schmidt process, but we saw earlier that alternatively we can use the three term recurrence relation.
- Choosing $Q_n$ this way our integral simplifies
\[ I = \int_{a}^{b} w(x)r(x)dx \]
\[ = \sum_{i=1}^{n} w_i p(x_i) \]
\[ = \sum_{i=1}^{n} w_i (Q_n(x_i)q(x_i) + r(x_i)) \]

- To simplify this further **pick the** \( x_i \) **to be the roots of** \( Q_n \). **We get**

\[ I = \int_{a}^{b} w(x)r(x)dx = \sum_{i=1}^{n} w_i r(x_i) \]

- Now note that

\[ r(x) = \sum_{i=1}^{n} r(x_i)L_i(x) \]

(where the \( L_i \) are the Lagrange basis functions) and that hence

\[ I = \int_{a}^{b} w(x) \sum_{i=1}^{n} r(x_i)L_i(x) \]
\[ = \sum_{i=1}^{n} r(x_i) \int_{a}^{b} w(x)L_i(x)dx \]
\[ =: w_i \]
• So we pick the $x_i$ to be the roots of $Q_n$, i.e.,

$$Q_n(x_i) = 0, \quad i = 1, \ldots, n$$

and

$$w_i = \int_a^b w(x)L_i(x)dx.$$

• putting it all together we get

\[ I = \int_a^b w(x)p(x)dx \]

\[ = \int_a^b w(x)(Q_n(x)q(x) + r(x))dx \]

\[ = \int_a^b w(x)r(x)dx \]

\[ = \int_a^b w(x)\sum_{i=1}^n r(x_i)L_i(x)dx \]

\[ = \sum_{i=1}^n r(x_i)\int_a^b w(x)L_i(x)dx \]

\[ = \sum_{i=1}^n w_i r(x_i) \]

\[ = \sum_{i=1}^n w_i(Q_n(x_i)q(x_i) + r_i(x)) \]

\[ = \sum_{i=1}^n w_i p(x_i) \]

for all polynomials $p$ of degree up to $2n - 1$. 
Roots of Orthogonal Polynomials

What if the roots of $Q_n$ are not simple and in $(a, b)$?

- They are simple and in $(a, b)$. We can see this as follows:

- Suppose $Q_n$ changes sign at points $z_1, z_2, \ldots, z_k$ in $(a, b)$. Since $Q_n$ is a polynomial of degree $n$ we know that $k \leq n$ and we want to show that $k \geq n$, which implies that $k = n$.

- Consider the integral

$$Z = \int_a^b w(x)Q_n(x)(x-z_1)(x-z_2)\times\ldots\times(x-z_k).$$

- We know that $Z \neq 0$ since the integrand never changes sign. (This is where the positivity of $w$ becomes important).

- On the other hand, $Z$ is the inner product of $Q_n$ and a polynomial of degree $k$. Thus $k$ must be at least $n$ since $Q_n$ is orthogonal to all polynomials of degree less than $n$.

- This implies our result: there are $n$ simple roots of $Q_n$ in $(a, b)$.
Numerical Example

• Suppose we want to compute

\[ I = \int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, dx \]

where \( f \) is a well-behaved function that is well approximated by a polynomial.

• Using the above ideas with the weight function

\[ w(x) = \frac{1}{\sqrt{1 - x^2}} \]

we get the formulas

\[ \int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, dx = \sum_{i=1}^{n} w_i f(x_i) + R_n \]

where

\[ x_i = \cos \left( \frac{(2i - 1)\pi}{2n} \right), \quad n = 1, \ldots, n \]

\[ w_i = \frac{\pi}{n} \]

\[ R_n = \frac{\pi}{(2n)!2^{2n-1}} f^{(2n)}(\xi). \]

• The following Table lists the factor \( A_n \) multiplying the derivative for small values of \( n \):
\[
\begin{array}{ll}
n & A_n \\
1 & \frac{\pi}{4} \\
2 & \frac{\pi}{192} \\
3 & \frac{\pi}{23,040} \\
4 & \frac{\pi}{5,160,960} \\
5 & \frac{\pi}{1,857,445,600} \\
\end{array}
\]

- It is evident that 4 or 5 points suffice to get the integral accurately for most applications.

- By comparison, if we were to use an open Newton-Cotes Formula we would need to evaluate at millions of points just to get a modest accuracy of \(10^{-3}\) or so.
There are many formulas in Abramowitz/Stegun, here are just a few examples.

Examples of Orthogonal Polynomials

Legendre Polynomials

$$(f, g) = \int_{-1}^{1} f(x)g(x)dx, \quad w(x) = 1, \quad [a, b] = [-1, 1]$$

$p_0 = 1$
$p_1 = x$
$p_2 = -1/2 + 3/2x^2$
$p_3 = 5/2x^3 - 3/2x$
$p_4 = 3/8 + 35/8x^4 - 15/4x^2$
$p_5 = 63/8x^5 - 35/4x^3 + 15/8x$
$p_6 = -5/16 + 231/16x^6 - 315/16x^4 + 105/16x^2$
$p_7 = 429/16x^7 - 693/16x^5 + 315/16x^3 - 35/16x$
$p_8 = 35/128 + 6435/128x^8 - 3003/32x^6 + 3465/64x^4 - 315/32x^2$
Figure 1. Legendre Polynomials.
Chebychev Polynomials

\[(f, g) = \int_{-1}^{1} \frac{1}{\sqrt{1 - x^2}} f(x)g(x)\,dx, \quad w(x) = \frac{1}{\sqrt{1 - x^2}}, \quad [a, b] = [-1, 1] \]

\[p_0 = 1\]
\[p_1 = x\]
\[p_2 = 2x^2 - 1\]
\[p_3 = 4x^3 - 3x\]
\[p_4 = 8x^4 - 8x^2 + 1\]
\[p_5 = 16x^5 - 20x^3 + 5x\]
\[p_6 = 32x^6 - 48x^4 + 18x^2 - 1\]
\[p_7 = 64x^7 - 112x^5 + 56x^3 - 7x\]
\[p_8 = 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1\]
Figure 2. Chebychev Polynomials.
Laguerre Polynomials

\[(f, g) = \int_0^\infty e^{-x} f(x) g(x) \, dx, \quad w(x) = e^{-x}, \quad [a, b] = [0, \infty)\]

\[\begin{align*}
p_0 &= 1 \\
p_1 &= 1 - x \\
p_2 &= 1 - 2x + 1/2x^2 \\
p_3 &= 1 - 3x + 3/2x^2 - 1/6x^3 \\
p_4 &= 1 - 4x + 3x^2 - 2/3x^3 + 1/24x^4 \\
p_5 &= 1 - 5x + 5x^2 - 5/3x^3 + 5/24x^4 - 1/120x^5 \\
p_6 &= 1 - 6x + 15/2x^2 - 10/3x^3 + 5/8x^4 - 1/20x^5 + 1/720x^6 \\
p_7 &= 1 - 7x + 21/2x^2 - 35/6x^3 + 35/24x^4 - 7/40x^5 + \\
&\quad 7/720x^6 - 1/5040x^7 \\
p_8 &= 1 - 8x + 14x^2 - 28/3x^3 + 35/12x^4 - 7/15x^5 \\
&\quad + 7/180x^6 - 1/630x^7 + 1/40320x^8
\end{align*}\]
Figure 3. Laguerre Polynomials.
Hermite Polynomials

\[(f, g) = \int_{-\infty}^{\infty} e^{-x^2} f(x) g(x) dx, \quad w(x) = e^{-x^2}, \quad (a, b) = (-\infty, \infty)\]

\[p_0 = 1\]
\[p_1 = 2x\]
\[p_2 = 4x^2 - 2\]
\[p_3 = 8x^3 - 12x\]
\[p_4 = 16x^4 - 48x^2 + 12\]
\[p_5 = 32x^5 - 160x^3 + 120x\]
\[p_6 = 64x^6 - 480x^4 + 720x^2 - 120\]
\[p_7 = 128x^7 - 1344x^5 + 3360x^3 - 1680x\]
\[p_8 = 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680\]
Figure 4. Hermite Polynomials.