III.6 Gaussian quadrature

In this chapter we see that a special quadrature rule can be constructed by using the roots of orthogonal polynomials, leading to a method that is exact for polynomials of twice the expected degree. Importantly, we can use quadrature to compute expansions in orthogonal polynomials that interpolate, mirroring the link between the Trapezium rule, Fourier series, and interpolation but now for orthogonal polynomials.

1. Truncated Jacobi matrices: we see that truncated Jacobi matrices are diagonalisable

in terms of orthogonal polynomials and their zeros. 2. Gaussian quadrature: Using roots of orthogonal polynomials and truncated Jacobi matrices leads naturally to an efficiently computable interpolatory quadrature rule. The *miracle* is its exact for twice as many polynomials as expected.

1. Roots of orthogonal polynomials and truncated Jacobi matrices

We now consider roots (zeros) of orthogonal polynomials $p_n(x)$. This is important as we shall see they are useful for interpolation and quadrature. For interpolation to be well-defined we first need to guarantee that the roots are distinct.

Lemma 1 An orthogonal polynomial $p_n(x)$ has exactly n distinct roots.

Proof

Suppose $x_1, \ldots, x_j$ are the roots where $q_n(x)$ changes sign, that is,

$$p_n(x) = c_k(x - x_k)^{2p+1} + O((x - x_k)^{2p+2})$$

for $c_k \neq 0$ and $k = 1, \ldots, j$ and $p \in \mathbb{Z}$, as $x \to x_k$. Then

$$p_n(x)(x - x_1) \cdots (x - x_j)$$

does not change signs: it behaves like $c_k(x - x_k)^{2p+2} + O(x - x_k)^{2p+3}$ as $x \to x_k$. In other words:

$$\langle p_n, (x - x_1) \cdots (x - x_j) \rangle = \int_a^b p_n(x)(x - x_1) \cdots (x - x_j) w(x) \mathrm{d}x \neq 0.$$

where $w(x)$ is the weight of orthogonality. This is only possible if $j = n$ as $p_n(x)$ is orthogonal w.r.t. all lower degree polynomials.

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Definition 1 (truncated Jacobi matrix) Given a symmetric Jacobi matrix X (associated with a family of orthonormal polynomials), the *truncated Jacobi matrix* is

$$J_n := \begin{bmatrix} a_0 & b_0 \\ b_0 & \ddots & \ddots \\ & \ddots & a_{n-2} & b_{n-2} \\ & & b_{n-2} & a_{n-1} \end{bmatrix} \in \mathbb{R}^{n\times n}$$

Lemma 2 (zeros) The zeros $x_1, \ldots, x_n$ of an orthonormal polynomial $q_n(x)$ are the eigenvalues of the truncated Jacobi matrix J_n. More precisely,

$$J_n Q_n = Q_n \begin{bmatrix} x_1 \\ & \ddots \\ & & x_n \end{bmatrix}$$

for the orthogonal matrix

$$Q_n = \underbrace{\begin{bmatrix} q_0(x_1) & \cdots & q_0(x_n) \\ \vdots & \cdots & \vdots \\ q_{n-1}(x_1) & \cdots & q_{n-1}(x_n) \end{bmatrix}}_{V_n^\top} \begin{bmatrix} \alpha_1^{-1} \\ & \ddots \\ & & \alpha_n^{-1} \end{bmatrix}$$

where $\alpha_j = \sqrt{q_0(x_j)^2 + \cdots + q_{n-1}(x_j)^2}$.

Proof

We construct the eigenvector (noting $b_{n-1} q_n(x_j) = 0$):

$$J_n \begin{bmatrix} q_0(x_j) \\ \vdots \\ q_{n-1}(x_j) \end{bmatrix} = \begin{bmatrix} a_0 q_0(x_j) + b_0 q_1(x_j) \\ b_0 q_0(x_j) + a_1 q_1(x_j) + b_1 q_2(x_j) \\ \vdots \\ b_{n-3} q_{n-3}(x_j) + a_{n-2} q_{n-2}(x_j) + b_{n-2} q_{n-1}(x_j) \\ b_{n-2} q_{n-2}(x_j) + a_{n-1} q_{n-1}(x_j) + b_{n-1} q_n(x_j) \end{bmatrix} = x_j \begin{bmatrix} q_0(x_j) \\ q_1(x_j) \\ \vdots \\ q_{n-1}(x_j) \end{bmatrix}$$

The result follows from normalising the eigenvectors. Since J_n is symmetric the eigenvector matrix is orthogonal.

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Example 1 (Chebyshev roots) Consider $T_n(x) = \cos n \operatorname{acos} x$. The roots are $x_j = \cos \theta_j$ where $\theta_j = (j - 1/2)\pi/n$ for $j = 1, \ldots, n$ are the roots of $\cos n\theta$ that are inside $[0, \pi]$.

Consider the $n = 3$ case where we have

$$x_1, x_2, x_3 = \cos(\pi/6), \cos(\pi/2), \cos(5\pi/6) = \sqrt{3}/2, 0, -\sqrt{3/2}$$

We also have from the 3-term recurrence:

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \\ T_2(x) = 2xT_1(x) - T_0(x) &= 2x^2 - 1 \\ T_3(x) = 2xT_2(x) - T_1(x) &= 4x^3 - 3x \end{aligned}$$

We orthonormalise by rescaling

$$\begin{aligned} q_0(x) &= 1/\sqrt{\pi} \\ q_k(x) &= T_k(x)\sqrt{2}/\sqrt{\pi} \end{aligned}$$

so that the Jacobi matrix is symmetric:

$$x[q_0(x)|q_1(x)|\cdots] = [q_0(x)|q_1(x)|\cdots] \underbrace{\begin{bmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/2 \\ & 1/2 & 0 & 1/2 \\ & & 1/2 & 0 & \ddots \\ & & & \ddots & \ddots \end{bmatrix}}_{X}$$

We can then confirm that we have constructed an eigenvector/eigenvalue of the 3×3 truncation of the Jacobi matrix, e.g. at $x_2 = 0$:

$$\begin{bmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/2 \\ & 1/2 & 0 \end{bmatrix} \begin{bmatrix} q_0(0) \\ q_1(0) \\ q_2(0) \end{bmatrix} = \frac{1}{\sqrt{\pi}} \begin{bmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/2 \\ & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ -\sqrt{2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

2. Gaussian quadrature

Gaussian quadrature is the interpolatory quadrature rule corresponding to the grid x_j defined as the roots of the orthonormal polynomial $q_n(x)$. We shall see that it is exact for polynomials up to degree $2n - 1$, i.e., double the degree of other interpolatory quadrature rules from other grids.

Definition 2 (Gauss quadrature) Given a weight $w(x)$, the Gauss quadrature rule is:

$$\int_a^b f(x)w(x)\mathrm{d}x \approx \underbrace{\sum_{j=1}^n w_j f(x_j)}_{\Sigma_n^w[f]}$$

where $x_1, \ldots, x_n$ are the roots of the orthonormal polynomials $q_n(x)$ and

$$w_j := \frac{1}{\alpha_j^2} = \frac{1}{q_0(x_j)^2 + \cdots + q_{n-1}(x_j)^2}.$$

Equivalently, $x_1, \ldots, x_n$ are the eigenvalues of J_n and

$$w_j = \int_a^b w(x) \mathrm{d}x Q_n[1, j]^2.$$

(Note we have $\int_a^b w(x) \mathrm{d}x q_0(x)^2 = 1$.)

In analogy to how Fourier series are orthogonal with respect to the Trapezium rule, Orthogonal polynomials are orthogonal with respect to Gaussian quadrature:

Lemma 3 (Discrete orthogonality) For $0 \le \ell, m \le n-1$, the orthonormal polynomials $q_n(x)$ satisfy

$$\Sigma_n^w[q_\ell q_m] = \delta_{\ell m}$$

Proof

$$\Sigma_n^w[q_\ell q_m] = \sum_{j=1}^n \frac{q_\ell(x_j) q_m(x_j)}{\alpha_j^2} = [q_\ell(x_1)/\alpha_1 | \cdots | q_\ell(x_n)/\alpha_n] \begin{bmatrix} q_m(x_1)/\alpha_1 \\ \vdots \\ q_m(x_n)/\alpha_n \end{bmatrix} = \mathbf{e}_\ell Q_n$$

$$\delta_{\ell m}$$

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Just as approximating Fourier coefficients using Trapezium rule gives a way of interpolating at the grid, so does Gaussian quadrature:

Theorem 1 (interpolation via quadrature) For the orthonormal polynomials $q_n(x)$,

$$f_n(x) := \sum_{k=0}^{n-1} c_k^n q_k(x) \text{ for } c_k^n := \Sigma_n^w[f q_k]$$

interpolates $f(x)$ at the Gaussian quadrature points $x_1, \ldots, x_n$.

Proof

Consider the Vandermonde-like matrix from above:

$$V_n := \begin{bmatrix} q_0(x_1) & \cdots & q_{n-1}(x_1) \\ \vdots & \ddots & \vdots \\ q_0(x_n) & \cdots & q_{n-1}(x_n) \end{bmatrix}$$

and define

$$Q_n^w := V_n^\top \begin{bmatrix} w_1 & & \\ & \ddots & \\ & & w_n \end{bmatrix} = \begin{bmatrix} q_0(x_1)w_1 & \cdots & q_0(x_n)w_n \\ \vdots & \ddots & \vdots \\ q_{n-1}(x_1)w_1 & \cdots & q_{n-1}(x_n)w_n \end{bmatrix}$$

so that

$$\begin{bmatrix} c_0^n \\ \vdots \\ c_{n-1}^n \end{bmatrix} = Q_n^w \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}.$$

Note that if $p(x) = [q_0(x)| \cdots |q_{n-1}(x)]\mathbf{c}$ then

$$\begin{bmatrix} p(x_1) \\ \vdots \\ p(x_n) \end{bmatrix} = V_n \mathbf{c}$$

But we see that (similar to the Fourier case)

$$Q_n^w V_n = \begin{bmatrix} \Sigma_n^w[q_0 q_0] & \cdots & \Sigma_n^w[q_0 q_{n-1}] \\ \vdots & \ddots & \vdots \\ \Sigma_n^w[q_{n-1} q_0] & \cdots & \Sigma_n^w[q_{n-1} q_{n-1}] \end{bmatrix} = I_n$$

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Example 2 (Chebyshev expansions) Consider the construction of Gaussian quadrature associated with the Chebyshev weight for $n = 3$. To determine the weights we need:

$$w_j^{-1} = \alpha_j^2 = q_0(x_j)^2 + q_1(x_j)^2 + q_2(x_j)^2 = \frac{1}{\pi} + \frac{2}{\pi} x_j^2 + \frac{2}{\pi}(2x_j^2 - 1)^2$$

We can check each case and deduce that $w_j = \pi/3$. Thus we recover the interpolatory quadrature rule. Further, we can construct the transform

$$\begin{aligned} Q_3^w &= \begin{bmatrix} w_1 q_0(x_1) & w_2 q_0(x_2) & w_3 q_0(x_3) \\ w_1 q_1(x_1) & w_2 q_1(x_2) & w_3 q_1(x_3) \\ w_1 q_3(x_1) & w_2 q_3(x_2) & w_3 q_3(x_3) \end{bmatrix} \\ &= \frac{\pi}{3} \begin{bmatrix} 1/\sqrt{\pi} & 1/\sqrt{\pi} & 1/\sqrt{\pi} \\ x_1\sqrt{2/\pi} & x_2\sqrt{2/\pi} & x_3\sqrt{2/\pi} \\ (2x_1^2-1)\sqrt{2/\pi} & (2x_2^2-1)\sqrt{2/\pi} & (2x_3^2-1)\sqrt{2/\pi} \end{bmatrix} \\ &= \frac{\sqrt{\pi}}{3} \begin{bmatrix} 1 & 1 & 1 \\ \sqrt{6}/2 & 0 & -\sqrt{6}/2 \\ 1/\sqrt{2} & -\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \end{aligned}$$

We can use this to expand a polynomial, e.g. x^2:

$$Q_3^w \begin{bmatrix} x_1^2 \\ x_2^2 \\ x_3^2 \end{bmatrix} = \frac{\sqrt{\pi}}{3} \begin{bmatrix} 1 & 1 & 1 \\ \sqrt{6}/2 & 0 & -\sqrt{6}/2 \\ 1/\sqrt{2} & -\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 3/4 \\ 0 \\ 3/4 \end{bmatrix} = \begin{bmatrix} \sqrt{\pi}/2 \\ 0 \\ \sqrt{\pi}/(2\sqrt{2}) \end{bmatrix}$$

In other words:

$$x^2 = \frac{\sqrt{\pi}}{2} q_0(x) + \frac{\sqrt{\pi}}{2\sqrt{2}} q_2(x) = \frac{1}{2} T_0(x) + \frac{1}{2} T_2(x)$$

which can be easily confirmed.

Corollary 1 Gaussian quadrature is an interpolatory quadrature rule with the interpolation points equal to the roots of q_n:

$$\Sigma_n^w[f] = \int_a^b f_n(x) w(x) \mathrm{d}x$$

Proof We want to show that its the same as integrating the interpolatory polynomial:

$$\int_a^b f_n(x) w(x) \mathrm{d}x = \frac{1}{q_0(x)} \sum_{k=0}^{n-1} c_k^n \int_a^b q_k(x) q_0(x) w(x) \mathrm{d}x = \frac{c_0^n}{q_0} = \Sigma_n^w[f].$$

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Example 3 (Chebyshev quadrature via Lagrange polynomials) The connection with interpolatory quadrature means theres another way to compute the quadrature: integrate the Lagrange polynomials associated with the zeros. For example, with $n = 3$ recall that the roots of $T_3(x)$ are $\pm\sqrt{3}/2$ and 0. Thus we have

$$\begin{aligned} \ell_1(x) &= x(x + \sqrt{3}/2)/(3/2) = \frac{(2x^2 + \sqrt{3}x)}{3} \\ \ell_2(x) &= (x - \sqrt{3}/2)(x + \sqrt{3}/2)/(-3/4) = -\frac{4}{3}x^2 + 1 \\ \ell_3(x) &= (x - \sqrt{3}/2)x/(3/2) = \frac{(2x^2 - \sqrt{3}x)}{3} \end{aligned}$$

A quick check confirms that

$$w_j = \int_{-1}^1 \frac{\ell_j(x)}{\sqrt{1 - x^2}} \mathrm{d}x = \frac{\pi}{3}.$$

A consequence of being an interpolatory quadrature rule is that it is exact for all polynomials of degree $n - 1$. The *miracle* of Gaussian quadrature is it is exact for twice as many!

Theorem 2 (Exactness of Gauss quadrature) If $p(x)$ is a degree $2n - 1$ polynomial then Gauss quadrature is exact:

$$\int_a^b p(x)w(x)\mathrm{d}x = \Sigma_n^w[p].$$

Proof Using polynomial division algorithm (e.g. by matching terms) we can write

$$p(x) = q_n(x)s(x) + r(x)$$

where s and r are degree $n-1$ and $q_n(x)$ is the degree n orthonormal polynomial. Then we have:

$$\begin{aligned}
\Sigma_n^w[p] &= \underbrace{\Sigma_n^w[q_n s]}_{0 \text{ since evaluating } q_n \text{ at zeros}} + \Sigma_n^w[r] = \int_a^b r(x)w(x)\mathrm{d}x \\
&= \underbrace{\int_a^b q_n(x)s(x)w(x)\mathrm{d}x}_{0 \text{ since } s \text{ is degree } < n} + \int_a^b r(x)w(x)\mathrm{d}x \\
&= \int_a^b p(x)w(x)\mathrm{d}x.
\end{aligned}$$

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Example 4 (Double exactness) We are exact for all polynomials of degree $2n-1$, so for our $n=3$ rule consider integrating x^5. We correctly get:

$$\Sigma_n^w[x^5] = \frac{\pi}{3}\left(\frac{9\sqrt{3}}{32} - \frac{9\sqrt{3}}{2}\right) = 0.$$

We are also correct for x^4:

$$\Sigma_n^w[x^4] = \frac{\pi}{3}\left(\frac{9}{16} + \frac{9}{16}\right) = \frac{3\pi}{8}.$$

However,

$$\Sigma_n^w[x^6] = \frac{9\pi}{64} \neq \frac{5\pi}{16}$$

hence it is incorrect for larger degree polynomials.