MATH50003
Numerical Analysis

VI.3 Gaussian Quadrature

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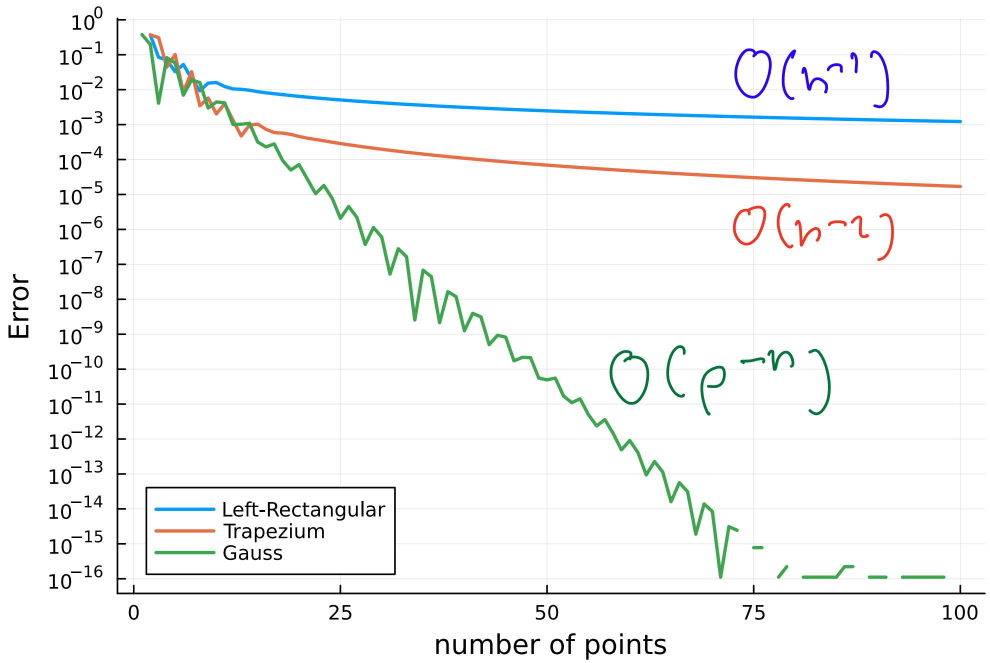
Part VI
Orthogonal Polynomials

1. General Orthogonal Polynomials and basic properties
2. Classical Orthogonal Polynomials with special structure
3. Gaussian Quadrature for high-accuracy integration

IV.5 Gaussian Quadrature = Interpolatory quadrature w/ roots of OP

Integrating with exponential convergence

$$\int_{-1}^{1} \frac{dx}{25(x-1/2)^2+1} \approx \sum_{j=1}^{n} w_j f(x_j)$$



algebraic

Exponential

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

Example 26 (Gauss-Chebyshev). Use roots of $T_n(x)$ for interp. quad.

$n=3$

Recall $T_3(x) = 4x^3 - 3x$, w/ roots

$x_2 = 0$, roots of

$$4x^2 - 3 = 0 \Rightarrow x_1 = -\frac{\sqrt{3}}{2}$$

$$x_3 = \frac{\sqrt{3}}{2}$$

We want to find w_1, w_2, w_3 so that

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \approx w_1 f(\underbrace{x_1}_{-\frac{\sqrt{3}}{2}}) + w_2 f(\underbrace{x_2}_{0}) + w_3 (\underbrace{x_3}_{\frac{\sqrt{3}}{2}})$$

How? use Lagrange basis.

Note (by trig subs.)

$$\int_{-1}^{1} \underbrace{w(x)}_{\frac{1}{\sqrt{1-x^2}}}\,dx = \pi, \quad \int_{-1}^{1} x\,w(x)\,dx \underset{\text{by symmetry}}{=} 0, \quad \int_{-1}^{1} x^2 w(x)\,dx = \frac{\pi}{2}.$$

We find

$$w_1 = \int_{-1}^{1} w(x)\,\underbrace{l_1(x)}_{\frac{x(x+\sqrt{3}/2)}{\sqrt{3}/2\,\sqrt{3}}}\,dx = \frac{\pi}{3}$$

$$w_2 = \int_{-1}^{1} w(x)\,\underbrace{l_2(x)}_{x^2-3/4}\,dx = \frac{\pi}{3}$$

Why? Special to Gauss-Chebyshev see PS.

$-3/4$

$$w_3 = \int_{-1}^{1} w(x)\, \ell_3(x)\, dx = \pi/3$$

$$\Rightarrow$$

$$\Sigma_n^{w,\tilde{x}}[f] = \frac{\pi}{3}\left[f\left(\frac{\sqrt{3}}{2}\right) + f(0) + f\left(-\frac{\sqrt{3}}{2}\right)\right]$$

Note

$$\Sigma_n^{w,\tilde{x}}[1] = \pi = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}}\, dx$$

$$\Sigma_n^{w}[x] = 0 = \int_{-1}^{1} \frac{x}{\sqrt{1-x^2}}\, dx$$

Guaranteed because interp.

$$\Sigma_n^{w}[x^2] = \frac{\pi}{3}\left(\frac{3}{4} + \frac{3}{4}\right) = \frac{\pi}{2} = \int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\, dx$$

$$\sum_n^w [x^3] = 0 = \int_{-1}^{1} \frac{x^3}{\sqrt{1-x^2}}\,dx$$

$$\sum_n^w [x^4] = \frac{3\pi}{8} = \int_{-1}^{1} \frac{x^4}{\sqrt{1-x^2}}\,dx$$

check

$$\sum_n^w [x^5] = 0 = \int_{-1}^{1} \frac{x^5}{\sqrt{1-x^2}}\,dx$$

up to degree $2n-1$ for free!

$$\sum_n^w [x^6] \neq \int_{-1}^{1} \frac{x^6}{\sqrt{1-x^2}}\,dx$$

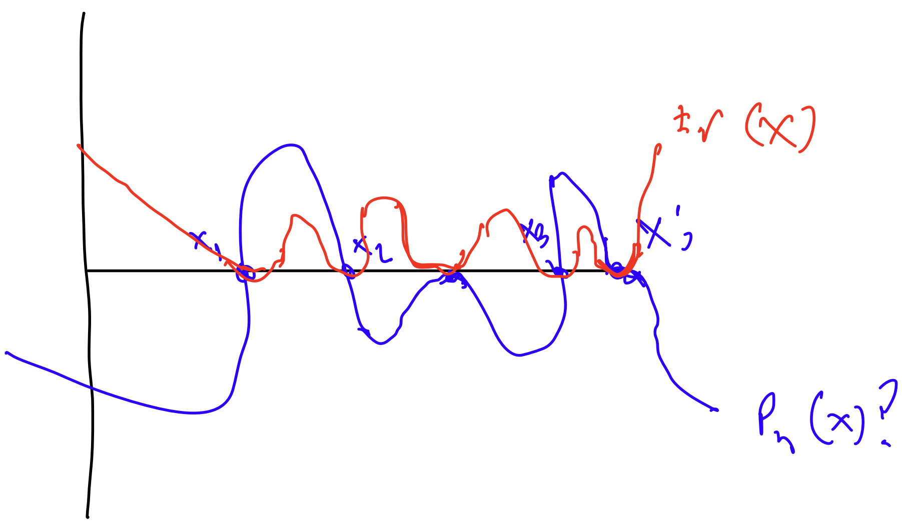
Why exact for degree $2n-1$?

VI.3.1 Roots of orthogonal polynomials and truncated Jacobi matrices

We can compute roots from eigenvalues

easy on a computer

Lemma 11 (OP roots). *An orthogonal polynomial $p_n(x)$ has exactly n distinct roots.*



Proof

Denote $x_1 - x_j$ roots where p_n changes sign. (odd multiplicity)

Near root:

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

$\Rightarrow$ $r(x) := P_n(x)(x-x_1) \cdots (x-x_j)$

does not change sign

$\Rightarrow$ $\langle P_n, (x-x_1) \cdots (x-x_j) \rangle =$

$$\int_a^b \underbrace{P_n(x)(x-x_1) \cdots (x-x_j)}_{r(x) > 0 \quad \text{or} \quad r(x) < 0} w(x)\,dx \neq 0$$

$\Rightarrow$ $(x-x_1) \cdots (x-x_j)$ is not degree $< n$

$\Rightarrow$ $j = n \Rightarrow$ all roots in this list.

Definition 42 (truncated Jacobi matrix)**.** Given a Jacobi matrix J associated with a family of orthonormal polynomials, the *truncated Jacobi matrix* is

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

Claim

$$J_n = \underbrace{Q_n}_{\text{in terms of OPs}} \underbrace{\Lambda}_{\begin{bmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{bmatrix}} Q_n^T$$

roots of $p_n(x)$

Lemma 12 (OP roots and Jacobi matrices)**.** *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

$$Q_n = \underbrace{\begin{array}{c} \begin{array}{ccc} \overbrace{\phantom{q_{n-1}(x_1)}}^{\vec{v}_1} & & \overbrace{\phantom{q_{n-1}(x_n)}}^{\vec{v}_n} \end{array} \\ \begin{bmatrix} q_0(x_1) & \cdots & q_0(x_n) \\ \vdots & \cdots & \vdots \\ q_{n-1}(x_1) & \cdots & q_{n-1}(x_n) \end{bmatrix} \end{array}}_{V_n^\top} \begin{bmatrix} \alpha_1^{-1} & & \\ & \ddots & \\ & & \alpha_n^{-1} \end{bmatrix} \in O(n)$$

where $\alpha_j = \underbrace{\sqrt{q_0(x_j)^2 + \cdots + q_{n-1}(x_j)^2}}_{\| \vec{v}_j \|}$.

Proof Show $\vec{v}_j$ are eigvec. w/ eigval x_j.

$$J_n \vec{v}_j = \begin{bmatrix} a_0 q_0(x_j) + b_0 q_1(x_j) \\ b_0 q_0(x_j) + a_0 q_1(x_j) + b_1 q_2(x_j) \\ \vdots \\ b_{n-3} q_{n-3}(x_j) + a_{n-2} q_{n-2}(x_j) + b_{n-2} q_{n-1}(x_j) \\ b_{n-2} q_{n-2}(x_j) + a_{n-1} q_{n-1}(x_j) + \underbrace{b_{n-1} q_n(x_j)}_{=0 \text{ at } x_j} \end{bmatrix}$$

$$\underset{\text{3-term}}{=} \begin{bmatrix} x_j q_0(x_j) \\ x_j q_1(x_j) \\ \vdots \\ x_j q_{n-1}(x_j) \end{bmatrix} = x_j \vec{v}_j$$

Example 27 (Chebyshev roots).

See note

what Gauss quad is to OPs

Trapezium rule is to Fourier

VI.3.2 Properties of Gaussian quadrature

Interpolatory quadrature rule associated with roots of OPs

Definition 43 (Gaussian quadrature)**.** Given a weight $w(x)$, the Gauss quadrature rule is:

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

will show is equivalent to interp,

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

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

$$= \int_a^b w(x)\mathrm{d}x \; \underbrace{\frac{q_0(x_j)^2}{\alpha_j^2}}$$

$Q_n[1, j+1]$

Gauss quad is defined in terms of eigen(J_n) & $\int_a^b w(x)\,dx$.

Lemma 13 (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

$$\Sigma_n^w[q_\ell q_m] \overset{\text{def}}{=} \sum_{j=1}^{n} \frac{q_\ell(x_j)\, q_m(x_j)}{\alpha_j^2}$$

$$= \underbrace{\begin{bmatrix} \frac{q_\ell(x_1)}{\alpha_1} \,\Big|\, \cdots \,\Big|\, \frac{q_\ell(x_n)}{\alpha_n} \end{bmatrix}}_{e_{\ell+1}^\top Q_n} \underbrace{\begin{bmatrix} q_m(x_1)/\alpha_1 \\ \vdots \\ q_m(x_n)/\alpha_n \end{bmatrix}}_{Q_n^\top e_{m+1}}$$

$$= e_{\ell+1}^\top \underbrace{Q_n Q_n^\top}\, e_{m+1} = \delta_{\ell m}$$

$= I$

Theorem 19 (interpolation via quadrature). *For the orthonormal polynomials* $q_n(x)$,

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

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

<u>Proof</u> Consider Vandermonde-like matrix

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

Define

$$Q_n^w := V_n^T \begin{bmatrix} w_1 & & \\ & \ddots & \\ & & w_n \end{bmatrix}$$

so that

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

But

$$Q_n^w V_n = \begin{bmatrix} \Sigma_n^w[a_0 a_0] & \cdots & \\ \vdots & \ddots & \\ \Sigma_n^w[a_{n-1} a_0] & \cdots & \Sigma_n^w[a_{n-1} a_{n-1}] \end{bmatrix}$$

$$= I$$

$$\Rightarrow \quad f_n(x_i) = \underbrace{\begin{bmatrix} q_0(x_i) & | & \cdots & | & q_{n-1}(x_i) \end{bmatrix}}_{e_i^T V_n} Q_n^w \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}$$

poly

$$= e_i^T V_n Q_n^w \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix} = f(x_i).$$

Example 28 (Chebyshev expansions).

See notes.

Corollary 11 (Gaussian quadrature is interpolatory)**.** *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 Follows immediately see notes.

Theorem 20 (Exactness of Gauss quadrature). *If $p(x)$ is a degree $2n-1$ polynomial then Gauss quadrature is exact:*

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

<u>Proof</u> Polynomial Division $\Rightarrow$

$$\underbrace{p(x)}_{\text{degree } 2n-1} = \underbrace{q_n(x)}_{\text{degree } n} \underbrace{s(x)}_{\text{degree } n-1} + \underbrace{r(x)}_{\text{degree } n-1}$$

$$\Rightarrow \Sigma_n^w[p] = \underbrace{\Sigma_n^w[q_n s]}_{=0} + \Sigma_n[r]$$

$$\stackrel{\text{interp.}}{=} \int_a^b r(x)\, w(x)\, dx$$

$$= \underbrace{\int_a^b q_n(x)\, s(x)\, w(x)\, dx}_{=0 \text{ since } s \text{ is degree } < n} + \int_a^b r(x)\, w(x)\, dx$$

$$= \int_a^b f(x)\, w(x)\, dx$$

∎

Example 29 (Double exactness).