

Quadrature

- For a given weight $w(x) \geq 0$, approximate the integral

$$\int f(x)w(x)dx \approx \sum_{j=0}^N w_j f(x_j)$$

Nodes (x_j)
Weights (w_j)

e.g. Jacobi weights

$$\int_{-1}^{+1} f(x)(1-x)^\alpha(1+x)^\beta dx$$

Or more generally,

- For Borel measures μ , approximate the integral

$$\int f(x)d\mu(x) \approx \sum_{j=0}^N w_j f(x_j)$$

$$\mu \approx \sum_{j=0}^N w_j \delta(\cdot - x_j)$$

e.g. For A self-adjoint $\exists!$ spectral measures μ_ℓ such that

$$f(A)_{\ell\ell} = \int f(x)d\mu_\ell$$

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Gauss Quadrature

- μ unit Borel measure on $\mathbb{R}$ & let $\{p_n\}$ be corresponding orthogonal polynomials:

$$p_n \in \mathcal{P}_n, \quad \int p_n(x)p_m(x)d\mu(x) = 0 \quad \text{for all } n \neq m \quad (1)$$

- Examples: Chebyshev I, II, Legendre, Two intervals I, II
- Nodes: Let $X_N = \{x_0, \dots, x_N\}$ be the set of zeros of p_{N+1}
(Need: nodes are distinct $\rightarrow$ proof later)
- Gauss quadrature:

$$\mathcal{I}_N f := \sum_{j=0}^N w_j f(x_j) := \int l_{X_N} f(x) d\mu(x)$$

where l_X is the polynomial interpolation on X

- That is, if $\ell_j(x) := \prod_{i \neq j} \frac{x-x_i}{x_j-x_i} \in \mathcal{P}_N$ (i.e. $\ell_j(x_i) = \delta_{ij}$), then
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 $w_j := \int \ell_j(x) d\mu(x)$,

$$\int P d\mu = \mathcal{I}_N P \text{ for all } P \in \mathcal{P}_{2N+1}$$

Proof: Take $P \in \mathcal{P}_{2N+1}$

- $\exists q_N, r_N \in \mathcal{P}_N$ such that $P = p_{N+1}q_N + r_N$,
- $P(x_j) = p_{N+1}(x_j)q_N(x_j) + r_N(x_j) = r_N(x_j)$

$$\begin{aligned} \int P d\mu &= \int [p_{N+1}q_N + r_N] d\mu \\ &= \int r_N d\mu && \text{(orthogonality)} \\ &= \int I_{X_N} r_N d\mu && (|X_N| = N + 1) \\ &= \sum_{j=0}^N w_j r_N(x_j) = \sum_{j=0}^N w_j P(x_j) \\ &= \mathcal{I}_N P \end{aligned}$$

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$$w_j \geq 0 \text{ and } \sum_{j=0}^N w_j = 1$$

Proof: Recall $\ell_j \in \mathcal{P}_N$ with $\ell_j(x_i) = \delta_{ij}$

- $\ell_j^2 \in \mathcal{P}_{2N}$ and so

$$0 \leq \int \ell_j^2 d\mu = \sum_{i=0}^N w_i \ell_j(x_i)^2 = w_j$$

- $P = \sum_{j=0}^N \ell_j \in \mathcal{P}_N$ with $P(x_j) = 1$ for $j = 0, \dots, N$,
- That is, $P(x) \equiv 1$ and so

$$\sum_{j=0}^N w_j = \sum_{j=0}^N w_j P(x_j) = \int P d\mu = \mu(\mathbb{R}) = 1$$

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Error estimates

Let $P \in \mathcal{P}_{2N+1}$,

$$\left| \int f d\mu - \mathcal{I}_N f \right| = \left| \int (f - P) d\mu + \mathcal{I}_N (P - f) \right| \quad (2)$$

$$\leq \int |f - P| d\mu + \sum_{j=0}^N w_j |f(x_j) - P(x_j)| \quad (3)$$

$$\leq 2 \|f - P\|_{L^\infty(\text{supp}(\mu) \cup X_N)} \quad (4)$$

Claim: number of points in X_N outside $\text{supp}(\mu)$ is bounded independently of N

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If $\text{supp}(\mu) \cap [a, b] = \emptyset$, then $|X_N \cap [a, b]| \leq 1$ - example

- Relabel so that $x_0, x_1 \in X_N \cap [a, b]$,
- Define $R(x) := \prod_{j=2}^N (x - x_j) \in \mathcal{P}_{N-1}$,
- Suppose $p_{N+1}(x) = c \prod_{j=0}^N (x - x_j)$,
- Since $(x - x_0)(x - x_1) > 0$ on $\text{supp } \mu$, we have

$$\int p_{N+1}(x) R(x) d\mu = c \int R(x)^2 (x - x_0)(x - x_1) d\mu \neq 0$$

- This contradicts the orthogonality property.

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$$\left| \int f d\mu - \mathcal{I}_N f \right| \leq 2 \inf_{P \in \mathcal{P}_{2N+1}} \|f - P\|_{L^\infty(\text{supp}(\mu) \cup X_N)} \quad (5)$$

$$\lesssim e^{-\gamma_N(2N+1)} \quad (6)$$

where $\gamma_N \rightarrow g_E(z^*)$ as $N \rightarrow \infty$ and z^* is the singularity of f “closest” to $\text{supp}(\mu)$

(c.f. logarithmic potential theory from last time I spoke)

What information about μ is needed to construct $\mathcal{I}_N$?

- i.e. what information is needed to construct p_{N+1} ?
- First $2N + 1$ moments

$$m_n := \int x^n d\mu(x) \quad \text{for } n = 1, \dots, 2N + 1$$

- In fact, can use Lanczos-type recursion to generate $\{p_n\}$:

$$p_{-1} := 0, \quad p_0 := 1, \quad \text{and} \quad a_0 := \int x d\mu = m_1, \quad b_0 := 0.$$

- Then for $n \geq 0$,

$$b_{n+1}p_{n+1} = (x - a_n)p_n(x) - b_n p_{n-1}(x)$$
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Summary

μ - unit Borel measure with compact support

Fix $E \subset \mathbb{R}$ compact
(under some conditions) $\exists!$ μ with moments m_n and support E

$$m_n = \int x^n d\mu(x) \\ \text{for } n = 0, \dots, 2N+1, \dots$$

$$\mu(x) = \frac{1}{2\pi} \lim_{\varepsilon \rightarrow 0} [G(x + i\varepsilon) - G(x - i\varepsilon)]$$

$$G(z) := [(T - z)^{-1}]_{00}$$

$$= \frac{1}{z - a_0 - \frac{b_1^2}{z - a_1 - \frac{b_2^2}{z - a_2 - \ddots}}}$$

$$T := \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & b_2 & \\ & b_2 & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$

$$T_N := \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & \ddots & \\ & \ddots & \ddots & b_N \\ & & b_N & a_N \end{pmatrix}$$

$$p_{n+1}(x) = c_n \begin{vmatrix} m_0 & m_1 & & m_n & m_{n+1} \\ m_1 & & m_n & m_{n+1} & \\ & m_n & m_{n+1} & & \\ m_n & m_{n+1} & & & m_{2n+1} \\ 1 & x & \dots & \dots & x^{n+1} \end{vmatrix}$$

OPs $p_0, \dots, p_{N+1}, \dots$

$$X_N := \{\text{roots of } p_{N+1}\} = \sigma(T_N)$$

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$$T := \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & b_2 & \\ & b_2 & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$

$$T_N := \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & \ddots & \\ & \ddots & \ddots & b_N \\ & & b_N & a_N \end{pmatrix}$$

$$p_{n+1}(x) = c_n \begin{vmatrix} m_0 & m_1 & & m_n & m_{n+1} \\ m_1 & & m_n & m_{n+1} & \\ & m_n & m_{n+1} & & \\ m_n & m_{n+1} & & & m_{2n+1} \\ 1 & x & \dots & \dots & x^{n+1} \end{vmatrix}$$

OPs $p_0, \dots, p_{N+1}, \dots$

$$X_N := \{\text{roots of } p_{N+1}\} = \sigma(T_N)$$

X_N - set of $N + 1$ distinct points

Proof: Since $\sigma(T_N) = X_N$ and $b_n > 0$ for each n , for each $\lambda \in X_N$, the matrix

$$T_N - \lambda = \begin{pmatrix} a_0 - \lambda & b_1 & & & \\ b_1 & a_1 - \lambda & b_2 & & \\ & b_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_N \\ & & & b_N & a_N - \lambda \end{pmatrix}$$

has full rank. Therefore, λ is a simple eigenvalue.

Spectral measures

- H bounded self-adjoint operator on a Hilbert space (e.g. symmetric real valued matrices)
- $\exists!$ μ_ℓ *spectral measure* such that

$$f(H)_{\ell\ell} = \int f \, d\mu_\ell$$

- $f(H)_{\ell\ell}$ is a local quantity of interest,
- Gauss quadrature leads to the nonlinear approximation

$$f(H)_{\ell\ell} \approx \sum_{j=0}^N w_j f(x_j) = g_N(H_{\ell\ell}, [H^2]_{\ell\ell}, \dots, [H^{2N+1}]_{\ell\ell})$$

where $g_N: U_N \subset \mathbb{C}^{2N+1} \rightarrow \mathbb{C}$ is analytic

- c.f. “linear” body order expansion

$$f(H)_{\ell\ell} \approx P_{2N+1}(H)_{\ell\ell} = \sum_{n=0}^{2N+1} c_n [H^n]_{\ell\ell}$$

Error estimates: comparison

- linear:

$$|f(H)_{\ell\ell} - P_{2N+1}(H)_{\ell\ell}| \leq \|f - P_{2N+1}\|_{L^\infty(\sigma(H))}$$

Problem: to obtain good estimates, we require knowledge of the point spectrum!

- nonlinear:

$$\left| f(H)_{\ell\ell} - \sum_{j=0}^N w_j f(x_j) \right| \leq 2 \inf_{P \in \mathcal{P}_{2N+1}} \|f - P\|_{L^\infty(\sigma(H) \cup X_N)}$$

where $|X_N \setminus \sigma(H)|$ bounded independently of N .

- Can use the potential theory results to bound the right hand sides (talked about this last time)

If $\text{supp}(\mu) \cap [a, b] = \emptyset$, then $|X_N \cap [a, b]| \leq 1$ - go back

