Quadrature

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

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

Nodes (x_j)
Weights (w_j)

e.g. Jacobi weights

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

Or more generally,

- For Borel measures μ, approximate the integral

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

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

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

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

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Gauss Quadrature

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

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

- 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 $\to$ proof later)
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$$\mathcal{I}_N f := \sum_{j=0}^{N} w_j f(x_j) := \int I_{X_N} f(x) \mathrm{d}\mu(x)$$

where I_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 $w_j := \int \ell_j(x) \mathrm{d}\mu(x)$,

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$\int P \mathrm{d}\mu = \mathcal{I}_N P$ 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 $P = p_{N+1} q_N + r_N$,
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$$\begin{aligned}
\int P \mathrm{d}\mu &= \int [p_{N+1} q_N + r_N] \mathrm{d}\mu \\
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&= \int I_{X_N} r_N \mathrm{d}\mu && (|X_N| = N+1) \\
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- $P = \sum_{j=0}^N \ell_j \in \mathcal{P}_N$ with $P(x_j) = 1$ for $j = 0, \ldots, N$,
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Error estimates

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

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

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

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

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

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If $\operatorname{supp}(\mu) \cap [a,b] = \emptyset$, 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 $\operatorname{supp}\mu$, we have

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

- This contradicts the orthogonality property.

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

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

where $\gamma_N \to g_E(z^\star)$ as $N \to \infty$ and $z^\star$ is the singularity of f "closest" to $\mathrm{supp}(\mu)$

(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

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

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

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

- Then for $n \geq 0$,

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μ - unit Borel measure with compact support

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

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

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

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

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

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μ - unit Borel measure with compact support

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

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

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

$$G(z) := \left[(T - z)^{-1} \right]_{00} = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \ddots}}}$$

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

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

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

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

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 eigenvlaue.

Spectral measures

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

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

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

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

  where $g_N \colon U_N \subset \mathbb{C}^{2N+1} \to \mathbb{C}$ 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 $\mathrm{supp}(\mu) \cap [a, b] = \emptyset$, then $|X_N \cap [a, b]| \leq 1$ - go back