Gauss quadrature and Lanczos algorithm

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Outline

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2. How to generalize Gauss quadrature?
3. Gauss quadrature and Lanczos algorithm
4. Jordan decomposition of complex Jacobi matrices

1. Polynomials orthogonal with respect to a linear functional

References:

T.S. Chihara, *An Introduction to Orthogonal Polynomials*, 1978

1 Linear functionals on polynomials

- $\mathcal{P}_n$ - the space of polynomials of degree up to n
- $\mathcal{L}$ - a linear functional on $\mathcal{P}_n$
- $\mathcal{L}$ is fully determined by its moments $m_j = \mathcal{L}(x^j)$, $j = 0, 1, \dots, n$.
- Any sequence of $n + 1$ complex numbers can be seen as a linear functional on $\mathcal{P}_n$.
- Hankel matrices of moments

$$M_j = \begin{bmatrix} m_0 & m_1 & \dots & m_j \\ m_1 & m_2 & \dots & m_{j+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_j & m_{j+1} & \dots & m_{2j} \end{bmatrix}$$

- $\Delta_j = det(M_j)$

- $\mathcal{L}$ is said to be positive definite on $\mathcal{P}_n$ if:
  1. $m_0, \ldots, m_{2n}$ are real,
  2. $\Delta_0, \ldots, \Delta_n$ are positive.

- There exists a distribution function μ such that

$$\mathcal{L}(p) = \int p(x) d\mu(x) \quad \text{for} \quad p \in \mathcal{P}_n.$$

- Bilinear form $[p, q] = \mathcal{L}(p\,q)$ is an inner product on $\mathcal{P}_n$.

- $\mathcal{L}$ is said to be quasi-definite on $\mathcal{P}_n$ if $\Delta_0, \ldots, \Delta_n$ are different from zero.

1 Orthogonal polynomials w.r. to quasi definite $\mathcal{L}$

- $\pi_0, \pi_1, \ldots$ is a sequence of orthogonal polynomials w.r. to $\mathcal{L}$ if:
  1. $\deg(\pi_j) = j$ (π_j is of degree j),
  2. $\mathcal{L}(\pi_i \, \pi_j) = 0$, $i < j$,
  3. $\mathcal{L}(\pi_j^2) \neq 0$.
- Sequence $\pi_0, \ldots, \pi_n$ of orthogonal polynomials w.r. to $\mathcal{L}$ exists if and only if $\mathcal{L}$ is quasi definite on $\mathcal{P}_n$.
- OPs are unique up to constant factor.
- OPs satisfy three-term recurrence relation

$$xp_i(x) = \gamma_i p_{i-1}(x) + \alpha_i p_i(x) + \beta_{i+1} p_{i+1}(x)$$

1 Three-term recurrence relation for orthogonal polynomials

- $$x \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} = T_n \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} + \beta_n \begin{bmatrix} 0 \\ 0 \\ \vdots \\ p_n(x) \end{bmatrix}$$

- $$T_n = \begin{bmatrix} \alpha_0 & \beta_1 & & & \\ \gamma_1 & \alpha_1 & \beta_2 & & \\ & \gamma_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & \gamma_{n-1} & \alpha_{n-1} \end{bmatrix}$$

- $\beta_i \neq 0$, $\gamma_i \neq 0$, for $i = 1, \ldots, n$

- $\beta_i = \gamma_i$ if OPs are normalized (T_n is complex Jacobi matrix)

2. How to generalize the Gauss quadrature?

References:

S. Pozza, M. P., Z. Strakoš, *Gauss quadrature for quasi-definite linear functionals*, IMA J. Numer. Anal. 37 (2017)

- $\mathcal{L}$ is positive definite on $\mathcal{P}_n$
- $$\mathcal{L}(f) \approx \sum_{k=1}^{n} \omega_k \, f(\lambda_k)$$
- The nodes λ_k are zeros of the nth orthogonal polynomial.
- The weights are given by the formula for the interpolatory quadrature.
- Computations are done differently.

2 Properties of the (classical) Gauss quadrature

- G1: the n-node Gauss quadrature attains the maximal algebraic degree of exactness $2n-1$.

- G2: it is well-defined and it is unique. Moreover, Gauss quadratures with a smaller number of nodes also exist and they are unique.

- G3: the n-node Gauss quadrature of a function f can be written in the form

$$m_0 \, \mathbf{e}_1^T f(J_n) \mathbf{e}_1,$$

  where J_n is the Jacobi matrix containing the coefficients from the three-term recurrence relation for orthonormal polynomials associated with $\mathcal{L}$;
  $m_0 = \mathcal{L}(x^0)$.
  We do not have to use orthonormal polynomials.

- $$\mathcal{L}(f) = \sum_{i=1}^{\ell} \sum_{h=0}^{s_i-1} A_{i,h}\, f^{(h)}(z_i) + R_n(f), \qquad n = s_1 + \ldots + s_\ell$$
- Its degree of exactness is at least $2n-1$ if and only if:
  1. it is exact on $\mathcal{P}_{n-1}$
  2. $(x-z_1)^{s_1}(x-z_2)^{s_2}\ldots(x-z_\ell)^{s_\ell}$ is nth orthogonal polynomial with respect to $\mathcal{L}$
- quadrature $= \mathcal{L}(H_{n-1})$
- H_{n-1} - the interpolating polynomial of f in the nodes z_i of multiplicities s_i
- Should we call it Gauss quadrature? (G1, G2 and G3)

Theorem

There exists the quadrature of form

$$\mathcal{L}(f) = \sum_{i=1}^{\ell} \sum_{j=0}^{s_i - 1} \omega_{i,j}\, f^{(j)}(\lambda_i) + R_n(f)$$

satisfying all three properties G1, G2 and G3

if and only if

$\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$.

3. Gauss quadrature and Lanczos algorithm

References:

S. Pozza, M. P., Z. Strakoš, *Lanczos algorithm and the complex Gauss quadrature*, 2017, submitted

- Input: $A, \mathbf{v}, \mathbf{w}$
- $\tilde{\mathcal{L}}(f) = \mathbf{w}^* f(A)\mathbf{v}$
- After n steps of Lanczos we have computed:

$$T_n, \quad \mathbf{v}_j = \phi_j(A)\,\mathbf{v}, \quad \mathbf{w}_j, \quad j = 0, \dots, n-1.$$

- ϕ_j are orthogonal polynomials w.r. to $\tilde{\mathcal{L}} \Rightarrow$

$$m_0\,\mathbf{e}_1^T f(T_n)\mathbf{e}_1 \quad \text{is the Gauss quadrature for } \tilde{\mathcal{L}}$$

- It is possible to perform n steps of Lanczos if and only if $\tilde{\mathcal{L}}$ is quasi-definite on $\mathcal{P}_n$.
- There is a breakdown in the step n if and only if

$$\Delta_j \neq 0, \quad j = 0, \dots, n, \quad \Delta_{n+1} = 0.$$

- If the quasi-definite linear functional on $\mathcal{P}_n$ is given by $\tilde{\mathcal{L}}(f) = \mathbf{w}^* f(A)\mathbf{v}$, then the corresponding Gauss quadrature can be constructed by performing n steps of the Lanczos algorithm. For such functionals we can say that the Lanczos algorithm is a matrix formulation of the Gauss quadrature.

- *Can we say the same for any linear functional $\mathcal{L}$ quasi-definite on $\mathcal{P}_n$?*
In order to construct the n-weight Gauss quadrature for $\mathcal{L}$, one needs only the first $2n$ moments m_k of $\mathcal{L}$, $k = 0, \ldots, 2n-1$.

  In general, there always exist a square matrix A and vectors $\mathbf{v}$ and $\mathbf{w}$ such that

$$\mathbf{w}^* A^k \mathbf{v} = m_k, \quad k = 0, \ldots, 2n-1.$$

3 Any Gauss quadrature can be obtained by Lanczos algorithm

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3 Linear functionals with real moments

- Let the moments $m_0, \ldots, m_{2n-1}$ of quasi-definite $\mathcal{L}$ be real.
- $f : \mathbb{R} \longrightarrow \mathbb{R}$
- The nodes and weights in GQ for $\mathcal{L}$ can be complex numbers.
- Is it a problem?
- If the input $A, \mathbf{v}, \mathbf{w}$ of Lanczos algorithm is real, then it is possible to avoid complex number computation, i.e., the number

$$m_0 \, \mathbf{e}_1^T f(T_n) \mathbf{e}_1$$

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Theorem

Let $\mathcal{L}$ be a quasi-definite linear functional on $\mathcal{P}_n$ whose moments $m_0, \ldots, m_{2n-1}$ are real, and let $\mathcal{G}_n$ be associated Gauss quadrature

$$\mathcal{G}_n(f) = \sum_{i=1}^{\ell} \sum_{j=0}^{s_i - 1} \omega_{i,j} \, f^{(j)}(\lambda_i).$$

Then the following holds:

1. For each $\lambda_i \notin \mathbb{R}$ with multiplicity s_i there is a node $\lambda_m = \overline{\lambda}_i$ with the same multiplicity.
2. For every $\lambda_i \in \mathbb{R}$ we have that $\omega_{i,j} \in \mathbb{R}$, for $j = 0, \ldots, s_i - 1$. If $\lambda_i \notin \mathbb{R}$ and $\lambda_m = \overline{\lambda}_i$, then $\omega_{m,j} = \overline{\omega}_{i,j}$ for $j = 0, \ldots, s_i - 1$.
3. If $f : \mathbb{R} \longrightarrow \mathbb{R}$ is such that $f^{(j)}(\bar{\lambda}_i) = \overline{f^{(j)}(\lambda_i)}$ for $i = 1, \ldots, \ell$ and $j = 0, \ldots, s_i - 1$, then $\mathcal{G}_n(f)$ is a real number.

4. Jordan decomposition of complex Jacobi matrices

References:

S. Pozza, M. P., Z. Strakoš, *Lanczos algorithm and the complex Gauss quadrature*, 2017, submitted

The columns $\mathbf{w}_t$, $t = 1, \ldots, n$, of the matrix W and the rows $\mathbf{v}_t$ of W^{-1} in the Jordan decomposition of the complex Jacobi matrix

$$J_n = W \, \Lambda \, W^{-1}$$

can be expressed in terms of nodes and weights in the Gauss quadrature and orthonormal polynomials p:

$$\mathbf{w}_t = \mathbf{w}^{(i,j)} = \frac{1}{j!} \begin{bmatrix} \mathbf{0}_j \\ p_j^{(j)}(\lambda_i) \\ \vdots \\ p_{n-1}^{(j)}(\lambda_i) \end{bmatrix}, \quad \mathbf{v}_t = \mathbf{v}^{(i,j)} = \sum_{k=j}^{s_i - 1} k! \, \omega_{i,k} \, \mathbf{w}^{(i,k-j)},$$

where i is a unique integer between 1 and ℓ, and j is a unique integer between 0 and $s_i - 1$, such that $t = s_0 + s_1 + \cdots + s_{i-1} + j + 1$ with $s_0 = 0$.

Concluding remarks

- Gauss quadrature can be naturally generalized to approximate quasi-definite linear functionals, where the interconnections with orthogonal polynomials and Lanczos algorithm are analogous to those in the positive definite case.

- Lanczos algorithm is a matrix formulation for GQ.

- The loss with respect to the positive definite case:
  1. the nodes can be complex and multiple (real and simple)
  2. the weights can be complex (positive)

Thank you very much for your attention!