Complex Jacobi Matrices and Gauss Quadrature for Quasi-definite Linear Functionals

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The Gauss quadrature can be formulated as a method for approximation of positive definite linear functionals. The underlying theory connects several classical topics including orthogonal polynomials and (real) Jacobi matrices. In [4] we investigated the problem of generalizing the concept of Gauss quadrature for approximation of linear functionals which are not positive definite. We showed that the concept can be generalized to quasi-definite functionals and based on a close relationship with orthogonal polynomials and complex Jacobi matrices.

Orthogonal polynomials

First we recall the basic theory of orthogonal polynomials ([2]). Let $\mathcal{L} : \mathcal{P} \rightarrow \mathbb{C}$ be a linear functional defined on the space of complex polynomials $\mathcal{P}$.

Definition 1 A sequence of polynomials $p_0, p_1, \dots, p_k$ such that $\deg(p_j) = j$ (p_j is of degree j), $\mathcal{L}(p_i p_j) = 0$, $i < j$ and $\mathcal{L}(p_j^2) \neq 0$, is called a sequence of orthogonal polynomials with respect to the linear functional $\mathcal{L}$.

We say *moments* of a linear functional the values $\mathcal{L}(x^i) = m_i$, for $i = 0, 1, \dots$. We define the *Hankel determinants* Δ_j of the matrices of moments as

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

Definition 2 A linear functional $\mathcal{L}$ for which the first $k+1$ Hankel determinants are nonzero, i.e., $\Delta_j \neq 0$ for $j = 0, 1, \dots, k$, is called quasi-definite on the space of polynomials $\mathcal{P}_k$ of degree at most k .

The linear functional $\mathcal{L}$ is said to be positive definite on $\mathcal{P}_k$ if $m_s \in \mathbb{R}$ for $s = 0, \dots, 2k$ and $\Delta_j > 0$ for $j = 0, \dots, k$. Moreover, there exists a positive non-decreasing distribution function μ supported on the real axis such that $\mathcal{L}(p) = \int p(x) d\mu(x)$ for all p from $\mathcal{P}_{2k}$. Hence, positive definite linear functionals are considered by the classic theory of Gauss quadrature.

Any sequence of *orthogonal polynomials* $p_0, p_1, \dots$ satisfies the three term recurrence relationship (see [2, p. 19]) which can be written in the matrix form

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

T_n is a tridiagonal complex matrix.

The eigenvalues of T_n are the zeros of p_n

If we consider a sequence of orthonormal polynomials, i.e., such that $\mathcal{L}(p_i^2) = 1$ for $i = 0, \dots, n-1$, then T_n is a symmetric matrix.

$$\text{for } f \in \mathcal{P}_{2n-1}, \quad \mathcal{L}(f) = \mathbf{e}_1^T f(J_n) \mathbf{e}_1 = \sum_{i=1}^{\ell} \sum_{j=0}^{s_i-1} \omega_{i,j} f^{(j)}(\lambda_i)$$

Unicity

Theorem 5 Let $\mathcal{L}$ be an arbitrary linear functional on $\mathcal{P}$. The n -weight quadrature (2) of degree of exactness at least $2n-1$ exists and is unique if and only if the n -th Hankel determinant is nonzero, i.e., $\Delta_{n-1} \neq 0$.

Jacobi matrices

We define *Jacobi matrix* the complex matrix

$$J_n = \begin{bmatrix} \alpha_0 & \beta_1 & & \\ \beta_1 & \alpha_1 & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix}.$$

with $\beta_i \neq 0$ for $i = 1, \dots, n-1$ (see [1]).

A real J_n is diagonalizable and has distinct eigenvalues.

If J_n is complex we have the following statements.

Theorem 1 Every tridiagonal matrix $T \in \mathbb{C}^{n \times n}$ with nonzero elements on its super-diagonal (or sub-diagonal) is non-derogatory, i.e., its eigenvalues have geometric multiplicity 1.

A complex J_n is diagonalizable if and only if it has distinct eigenvalues.

We proved the following theorem for the case of a quasi-definite linear functional.

Theorem 2 [Moment Matching Property] Let $\mathcal{L}$ be a quasi-definite linear functional on $\mathcal{P}_n$ and let J_n be the Jacobi matrix of coefficients from the recurrence relations for orthogonal polynomials with respect to $\mathcal{L}$. Then

$$\mathcal{L}(x^i) = m_0 \mathbf{e}_1^T (J_n)^i \mathbf{e}_1, \quad i = 0, \dots, 2n-1,$$

where $m_0 = \mathcal{L}(x^0)$.

Exactness

Finally, the following theorem gives the condition under which the degree of exactness of (2) is exactly $2n-1$ (i.e., it does not exceed $2n-1$). This issue has no counterpart in the positive-definite case where the n -node Gauss quadrature cannot have algebraic degree of exactness larger than $2n-1$.

Theorem 6 Let $\mathcal{L}$ be an arbitrary linear functional on $\mathcal{P}$ and let the n -weight quadrature (2) has degree of exactness at least $2n-1$. Then the degree of exactness of the quadrature (2) is (exactly) $2n-1$ if and only if the $(n+1)$ -st Hankel determinant is nonzero, i.e., $\Delta_n \neq 0$.

Quadrature rule

Positive definite linear functionals naturally lead to the well-known Gauss quadrature. Let us recall some of its basic properties:

- G1: The n -node Gauss quadrature attains the maximal algebraic degree of exactness $2n-1$.
- G2: The n -node Gauss quadrature is well-defined and it is unique. Naturally, the Gauss quadratures with a smaller number of nodes also exist and they are unique.
- G3: The Gauss quadrature of the 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 $\mathcal{L}$; $m_0 = \mathcal{L}(x^0)$.

The nodes of the Gauss quadrature are the eigenvalues of J_n and the weights are given by interpolation.

In [4] we revisit the situation for the functional $\mathcal{L}$ that is only quasi-definite. We start with the usual form of an n -node quadrature

$$\mathcal{L}(f) = \sum_{i=1}^n \omega_i f(\lambda_i) + R_n(f), \quad (1)$$

where the nodes $\lambda_1, \dots, \lambda_n$ are distinct and the last term stands for the quadrature error.

Theorem 3 The quadrature (1) is exact for every f from $\mathcal{P}_{2n-1}$ if and only if it is interpolatory and the polynomial

$$\varphi_n(x) = \prod_{i=1}^n (x - \lambda_i)$$

satisfies $\mathcal{L}(\varphi_n p) = 0$ for every $p \in \mathcal{P}_{n-1}$.

The quadrature rule (1) has the properties G1 and G2 if and only if

- $\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$
- $J_1, \dots, J_n$ are diagonalizable

In order to avoid this restriction we modify the quadrature considering the n -weight quadrature formula

$$\mathcal{L}(f) = \sum_{i=1}^{\ell} \sum_{j=0}^{s_i-1} \omega_{i,j} f^{(j)}(\lambda_i) + R_n(f), \quad (2)$$

where $n = s_1 + \dots + s_{\ell}$.

Theorem 4 Let $\mathcal{L}$ be an arbitrary linear functional on $\mathcal{P}$. The quadrature (2) is exact for every f from $\mathcal{P}_{2n-1}$ if and only if it is exact on $\mathcal{P}_{n-1}$ and the polynomial

$$\varphi_n(x) = (x - \lambda_1)^{s_1} (x - \lambda_2)^{s_2} \dots (x - \lambda_{\ell})^{s_{\ell}}$$

satisfies $\mathcal{L}(\varphi_n p) = 0$ for every $p \in \mathcal{P}_{n-1}$.

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

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