LANCZOS ALGORITHM AND THE COMPLEX GAUSS QUADRATURE

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Abstract. Gauss quadrature can be naturally generalized to approximate quasi-definite linear functionals, where the interconnections with (formal) orthogonal polynomials, Padé approximants, (complex) Jacobi matrices and Lanczos algorithm are analogous to those in the positive definite case. In this paper we show that existence of the n-weight (complex) Gauss quadrature corresponds to performing successfully the first n steps of the Lanczos algorithm for generating the biorthogonal bases of the two associated Krylov subspaces. We also prove that the Jordan decomposition of the (complex) Jacobi matrix can be explicitly expressed in terms of the Gauss quadrature nodes and weights and the associated orthogonal polynomials. Since the output of the Lanczos algorithm can be made real whenever the input is real, it can be shown that the value of the Gauss quadrature is a real number whenever all relevant moments of the quasi-definite linear functional are real.

Key words. Quasi-definite linear functionals, Gauss quadrature, orthogonal polynomials, complex Jacobi matrices, matching moments, Lanczos algorithm.

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1. Introduction.

We first briefly recall basic results on quasi-definite linear functionals and orthogonal polynomials; for more details we refer to [21] and the references given there.

Let $\mathcal{L}$ be a *linear* functional on the space $\mathcal{P}$ of polynomials with generally complex coefficients, $\mathcal{L} : \mathcal{P} \to \mathbb{C}$. The functional $\mathcal{L}$ is fully determined by its values on monomials, called moments,

$$\mathcal{L}(x^\ell) = m_\ell, \quad \ell = 0, 1, \dots,$$

with the associated Hankel determinants

$$\Delta_j = \begin{vmatrix} m_0 & m_1 & \dots & m_j \\ m_1 & m_2 & \dots & m_{j+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_j & m_{j+1} & \dots & m_{2j} \end{vmatrix}, \quad j = 0, 1, \dots. \tag{1.1}$$

In this paper we are interested in quasi-definite linear functionals.

DEFINITION 1.1. *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.*

A quasi-definite linear functional can be associated with a sequence of orthogonal polynomials uniquely determined up to multiplicative constants.

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Definition 1.2. *Polynomials $p_0, p_1, \dots$ satisfying the conditions*
1. *$deg(p_j) = j$ (p_j is of degree j),*
2. *$\mathcal{L}(p_i\, p_j) = 0$, $i < j$,*
3. *$\mathcal{L}(p_j^2) \neq 0$,*

form a sequence of orthogonal polynomials with respect to the linear functional $\mathcal{L}$. Orthogonal polynomials such that $\mathcal{L}(p_j^2) = 1$ are known as *orthonormal* polynomials.

Theorem 1.3 ([4, Chapter I, Theorem 3.1], [18, Chapter VII, Theorem 1]). *A sequence $\{p_j\}_{j=0}^{k}$ of orthogonal polynomials with respect to $\mathcal{L}$ exists if and only if $\mathcal{L}$ is quasi-definite on $\mathcal{P}_k$.*

A sequence of orthogonal polynomials $p_0, p_1, \dots$ satisfies the three-term recurrence relation of the form

$$\delta_j p_j(x) = (x - \alpha_{j-1}) p_{j-1}(x) - \gamma_{j-1} p_{j-2}(x), \quad \text{for} \quad j = 1, 2, \dots, \tag{1.2}$$

where we set $\gamma_0 = 0$, $p_{-1}(x) = 0$, $p_0(x) = c$ (c is a given complex number different from zero), and

$$\alpha_{j-1} = \frac{\mathcal{L}(x p_{j-1}^2)}{\mathcal{L}(p_{j-1}^2)},\ \delta_j = \frac{\mathcal{L}(x p_{j-1} p_j)}{\mathcal{L}(p_j^2)},\ \gamma_{j-1} = \frac{\mathcal{L}(x p_{j-2} p_{j-1})}{\mathcal{L}(p_{j-2}^2)},$$

(see [24, Theorem 3.2.1], [4, p. 19], [2, Theorem 2.4]). If the first $n+1$ polynomials $p_0, p_1, \dots, p_n$ exist, then all $\delta_1, \dots, \delta_n$ and $\gamma_1, \dots, \gamma_{n-1}$ are different from zero. The recurrence (1.2) for the first $n+1$ polynomials can be written in the matrix form

$$x \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} = T_n \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} + \delta_n \begin{bmatrix} 0 \\ 0 \\ \vdots \\ p_n(x) \end{bmatrix}, \tag{1.3}$$

where T_n is the irreducible tridiagonal complex matrix

$$T_n = \begin{bmatrix} \alpha_0 & \delta_1 & & \\ \gamma_1 & \alpha_1 & \ddots & \\ & \ddots & \ddots & \delta_{n-1} \\ & & \gamma_{n-1} & \alpha_{n-1} \end{bmatrix}.$$

We say that T_n is determined by the first $2n$ moments of $\mathcal{L}$. The $(2n+1)$st moment m_{2n} present in (1.1) for $j = n$ affects only the value of δ_n. Its value must assure that $\Delta_n \neq 0$; otherwise $\mathcal{L}(p_n^2) = 0$ and therefore p_n is not orthogonal polynomial with respect to $\mathcal{L}$.

A linear functional quasi-definite on $\mathcal{P}_n$ determines a family of irreducible tridiagonal matrices that are diagonally similar where this diagonal similarity is equivalent to rescaling the sequence of orthogonal polynomials. It is worth noting that any irreducible tridiagonal matrix is diagonally similar to a *symmetric* irreducible tridiagonal matrix, called *complex Jacobi matrix*. The properties of complex Jacobi matrices are summarized in [21, Section 4]. Here we recall the following result that is valid for any tridiagonal matrix T_n associated with a sequence (1.3) of orthogonal polynomials determined by a quasi-definite linear functional (see [21, Section 5]).

Theorem 1.4 (Moment Matching Property). *Let $\mathcal{L}$ be a quasi-definite linear functional on $\mathcal{P}_n$ and let T_n be given by (1.3). Then*

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

On the other hand, as shown in [4, Chapter I, Theorem 4.4], in the survey [19, Theorem 2.14] and firstly for the positive definite case by Favard in [5], if we consider any sequence of polynomials satisfying

$$d_j p_j(x) = (x - a_{j-1})p_{j-1}(x) - c_{j-1}p_{j-2}(x),\ j = 1, 2, \ldots, \tag{1.4}$$

where

$$p_{-1}(x) = 0,\ p_0(x) = c,\ c_0 = 0,\ a_j, d_j, c_j, c \in \mathbb{C},\ d_j, c_j, c \neq 0,$$

then there exists a quasi-definite linear functional $\mathcal{L}$ such that $p_0, p_1, \ldots,$ are orthogonal polynomials with respect to $\mathcal{L}$. In other words, providing that $c, d_j, c_j \neq 0$, polynomials generated by (1.4) are always orthogonal polynomials. In addition, they are orthonormal if and only if $c_j = d_j$ and p_0 is such that $\mathcal{L}(p_0^2) = 1$.

This also means that for any irreducible tridiagonal matrix T_n, there exists a linear functional $\mathcal{L}$ quasi-definite on $\mathcal{P}_{n-1}$ such that T_n is determined by the first $2n$ moments of $\mathcal{L}$. As shown, e.g, in [1, proof of Theorem 2.3], two irreducible tridiagonal matrices T_n and $\widehat{T}_n$ are determined by the first $2n$ moments of the same linear functional if and only if they are diagonally similar, i.e., if $T_n = D^{-1}\widehat{T}_n D$, where D is an invertible diagonal matrix. Or, equivalently, if and only if

$$\alpha_i = \hat{\alpha}_i, \quad i = 0, \ldots, n-1, \tag{1.5}$$

and

$$\delta_i\, \gamma_i = \hat{\delta}_i\, \hat{\gamma}_i, \quad i = 1, \ldots, n-1, \tag{1.6}$$

where the elements of $\widehat{T}_n$ are marked with a hat.

The paper examines the interconnection between the n-weight complex Gauss quadrature and the first n steps of the Lanczos algorithm for generating the biorthogonal bases of the two associated Krylov subspaces. It is organized as follows. In Section 2 we derive the Lanczos algorithm for generating biorthonormal bases for the spaces

$$\operatorname{span}\{\mathbf{v}, A\mathbf{v}, \ldots, A^{n-1}\mathbf{v}\} \quad \text{and} \quad \operatorname{span}\{\mathbf{w}, A^*\mathbf{w}, \ldots, (A^*)^{n-1}\mathbf{w}\}$$

from the well-known Stieltjes procedure for generating orthonormal polynomials with respect to the linear functional

$$\mathcal{L}(f) = \mathbf{w}^* f(A)\mathbf{v}. \tag{1.7}$$

If n is the maximal number of steps in the Lanczos algorithm that can be performed without breakdown, then there exists no complex Gauss quadrature in the sense of [21] for approximating the functional (1.7) with more than n weights. This is shown in Section 3. Section 4 shows that the rows of the matrix W^{-1} in the Jordan decomposition $J_n = W\,\Lambda\,W^{-1}$ of the complex Jacobi matrix J_n can be expressed as a linear combination of some particular generalized eigenvectors of J_n. The coefficients in these linear combinations are the Gauss quadrature weights. In Section 5 quasi-definite functionals with real moments are considered. Then the value of the Gauss quadrature is a real number. Using a proper scaling one can achieve that the Lanczos algorithm involves only real number computations.

Throughout the paper we deal with mathematical relationship between quantities that are determined exactly. Since the effects of rounding errors to computations using short recurrences are substantial, the results of this paper cannot be applied, without a thorough analysis, to finite precision computations. Such analysis is out of the scope of this paper. As in the positive definite case, however, understanding of the relationship assuming exact computation is a prerequisite for any further investigation.

2. Orthogonal polynomials and the Lanczos algorithm. Let A be a square complex matrix and let $\mathbf{v}$ be a complex vector of the corresponding dimension. The nth *Krylov subspace* generated by A and $\mathbf{v}$ is defined by

$$\mathcal{K}_n(A, \mathbf{v}) = \text{span}\{\mathbf{v}, A\mathbf{v}, \ldots, A^{n-1}\mathbf{v}\},$$

or, equivalently,

$$\mathcal{K}_n(A, \mathbf{v}) = \{p(A)\mathbf{v} : p \in \mathcal{P}_{n-1}\},$$

where $\mathcal{P}_{n-1}$ is the subspace of (all) polynomials of degree at most $n-1$. The basic facts about Krylov subspaces had been formulated by Gantmacher in 1934; see [6]. In particular, there exists a uniquely defined integer $d = d(A, \mathbf{v})$, called *the grade of* $\mathbf{v}$ *with respect to* A, so that the vectors $\mathbf{v}, \ldots, A^{d-1}\mathbf{v}$ are linearly independent and the vectors $\mathbf{v}, \ldots, A^{d-1}\mathbf{v}, A^d\mathbf{v}$ are linearly dependent. Clearly there exists a polynomial $p_d(\lambda)$ of degree d, called the minimal polynomial of $\mathbf{v}$ with respect to A, such that $p_d(A)\mathbf{v} = 0$. The other facts about Krylov subspaces can be found elsewhere; see, e.g, [17, Section 2.2].

For the given complex matrix A and $\mathbf{v} \neq 0, \mathbf{w} \neq 0$ complex vectors, consider the linear functional on the space of polynomials

$$\mathcal{L}(p) = \mathbf{w}^* p(A)\mathbf{v}. \tag{2.1}$$

Since for any polynomial p we get

$$p(A)^* = \bar{p}(A^*),$$

with $\bar{p}$ the polynomial whose coefficients are the conjugates of the coefficients of p, given $p, q \in \mathcal{P}_{n-1}$ we have

$$\mathcal{L}(pq) = \mathbf{w}^* q(A)p(A)\mathbf{v} = \hat{\mathbf{w}}^*\hat{\mathbf{v}},$$

with $\hat{\mathbf{v}} = p(A)\mathbf{v} \in \mathcal{K}_n(A, \mathbf{v})$ and $\hat{\mathbf{w}} = \bar{q}(A^*)\mathbf{w} \in \mathcal{K}_n(A^*, \mathbf{w})$.

THEOREM 2.1. *The linear functional $\mathcal{L}$ defined by (2.1) determines a sequence of orthogonal polynomials $p_0, \ldots, p_{n-1}$ if and only if there exist bases $\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}$ of $\mathcal{K}_n(A, \mathbf{v})$ and $\mathbf{w}_0 \ldots, \mathbf{w}_{n-1}$ of $\mathcal{K}_n(A^*, \mathbf{w})$ satisfying the biorthogonality condition*

$$\mathbf{w}_i^*\mathbf{v}_j = 0 \quad \textit{for } i \neq j, \qquad \textit{and} \qquad \mathbf{w}_i^*\mathbf{v}_i \neq 0, \;\; i, j = 0, \ldots, n-1. \tag{2.2}$$

Proof. Given polynomials $p_0, \ldots, p_{n-1}$ orthogonal with respect to $\mathcal{L}$, the vectors $\mathbf{v}_j = p_j(A)\mathbf{v}$ $(i = 0, \ldots, n-1)$ form the basis for $\mathcal{K}_n(A, \mathbf{v})$, vectors $\mathbf{w}_i = \bar{p}_i(A^*)\mathbf{w}$ form the basis for $\mathcal{K}_n(A^*, \mathbf{w})$, and

$$\mathbf{w}_i^*\mathbf{v}_j = \mathcal{L}(p_i p_j), \quad i, j = 0, \ldots, n-1,$$

Algorithm 2.2 (Stieltjes Procedure).
Input: linear functional $\mathcal{L}$ quasi-definite on $\mathcal{P}_{n-1}$.
Output: polynomials $\tilde{p}_0, \ldots, \tilde{p}_{n-1}$ orthonormal with respect to $\mathcal{L}$.

Initialize: $\tilde{p}_{-1} = 0, \beta_0 = \sqrt{m_0} = \sqrt{\mathcal{L}(x^0)}, \tilde{p}_0 = 1/\beta_0$.
For $j = 1, 2, \ldots, n-1$

$\alpha_{j-1} = \mathcal{L}(x\tilde{p}_{j-1}^2(x))$,

$\hat{p}_j(x) = (x - \alpha_{j-1})\tilde{p}_{j-1}(x) - \beta_{j-1}\tilde{p}_{j-2}(x)$,

$\beta_j = \sqrt{\mathcal{L}(\hat{p}_j^2)}$,

$\tilde{p}_j(x) = \hat{p}_j(x)/\beta_j$,

end.

satisfy the biorthogonality condition (2.2). On the other hand, let $\mathbf{v}_j = p_j(A)\mathbf{v}$ and $\mathbf{w}_i = \bar{q}_i(A^*)\mathbf{w}$ satisfy

$$\mathbf{w}_i^*\mathbf{v}_j = 0 \quad \text{for } i \neq j, \qquad \text{and} \qquad \mathbf{w}_i^*\mathbf{v}_i \neq 0, \;\; i, j = 0, \ldots, n-1,$$

and p_j and q_i are polynomials of degree j and i respectively. It means that the polynomial p_i is orthogonal to the polynomials $q_0, q_1, \ldots, q_{i-1}$, and therefore also to polynomials $p_0, p_1, \ldots, p_{i-1}$. The polynomial p_i is not orthogonal to q_i, and thus $\mathcal{L}(p_i^2) \neq 0$.□

We denote $\tilde{p}_0, \ldots, \tilde{p}_{n-1}$ the sequence of orthonormal polynomials with respect to $\mathcal{L}$. They satisfy the three-term recurrence relation

$$\beta_j\tilde{p}_j(x) = (x - \alpha_{j-1})\tilde{p}_{j-1}(x) - \beta_{j-1}\tilde{p}_{j-2}(x), \qquad j = 1, 2, \ldots, n-1, \tag{2.3}$$

with $\tilde{p}_{-1} = 0$, $\tilde{p}_0 = 1/\sqrt{m_0}$, and

$$\alpha_{j-1} = \mathcal{L}(x\tilde{p}_{j-1}^2), \;\; \beta_{j-1} = \mathcal{L}(x\tilde{p}_{j-2}\tilde{p}_{j-1}). \tag{2.4}$$

Note that $\beta_j = \sqrt{\mathcal{L}(\hat{p}_j^2)}$, with

$$\hat{p}_j(x) = (x - \alpha_{j-1})\tilde{p}_{j-1}(x) - \beta_{j-1}\tilde{p}_{j-2}(x). \tag{2.5}$$

Algorithm 2.2 generates the sequence of the first n orthonormal polynomials $\tilde{p}_j$, $j = 0, \ldots, n-1$, using the formulas (2.3) and (2.4). In order to avoid ambiguity, we take always the principal value of the complex square root, i.e., we consider $arg(\sqrt{c}) \in (-\pi/2, \pi/2]$. For positive definite functionals this algorithm is known as the Stieltjes procedure [23]. Then the coefficients β_j, $j = 1, \ldots, n-1$, are positive. The monograph by Gautschi [8] can serve as a valuable source of related results as well as of historical information.

The Lanczos algorithm (see [15] and [16]) gives the matrix formulation of the Stieltjes procedure. Indeed, with

$$\mathbf{v}_j = \tilde{p}_j(A)\mathbf{v}, \quad \mathbf{w}_j = \bar{\tilde{p}}_j(A^*)\mathbf{w}, \quad j = 0, \ldots, n-1,$$

Algorithm 2.3 (Lanczos algorithm).
Input: complex matrix A, two complex vectors $\mathbf{v}, \mathbf{w}$ such that $\mathbf{w}^*\mathbf{v} \neq 0$.
Output: vectors $\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}$ that span $\mathcal{K}_n(A, \mathbf{v})$ and vectors $\mathbf{w}_0, \ldots, \mathbf{w}_{n-1}$ that span $\mathcal{K}_n(A^*, \mathbf{w})$, satisfying the biorthogonality conditions (2.2).

Initialize: $\mathbf{v}_{-1} = \mathbf{w}_{-1} = 0$, $\beta_0 = \sqrt{\mathbf{w}^*\mathbf{v}}$
$\mathbf{v}_0 = \mathbf{v}/\beta_0$, $\mathbf{w}_0 = \mathbf{w}/\bar{\beta}_0$.
For $j = 1, 2, \ldots, n-1$
$\alpha_{j-1} = \mathbf{w}_{j-1}^* A \mathbf{v}_{j-1}$,
$\hat{\mathbf{v}}_j = A\mathbf{v}_{j-1} - \alpha_{j-1}\mathbf{v}_{j-1} - \beta_{j-1}\mathbf{v}_{j-2}$,
$\hat{\mathbf{w}}_j = A^*\mathbf{w}_{j-1} - \bar{\alpha}_{j-1}\mathbf{w}_{j-1} - \bar{\beta}_{j-1}\mathbf{w}_{j-2}$,
$\beta_j = \sqrt{\hat{\mathbf{w}}_j^* \hat{\mathbf{v}}_j}$,
if $\beta_j = 0$ *then stop,*
$\mathbf{v}_j = \hat{\mathbf{v}}_j/\beta_j$,
$\mathbf{w}_j = \hat{\mathbf{w}}_j/\bar{\beta}_j$,
end.

we have

$$\alpha_{j-1} = \mathcal{L}(x\tilde{p}_{j-1}^2) = \mathbf{w}^*\tilde{p}_{j-1}(A)A\tilde{p}_{j-1}(A)\mathbf{v} = \mathbf{w}_{j-1}^* A \mathbf{v}_{j-1},$$

for $j = 1, \ldots, n-1$. Since $\beta_j^2 = \mathcal{L}(\hat{p}_j^2(x))$ with the polynomial $\hat{p}_j$ defined by (2.5), we get

$$\beta_j = \sqrt{\mathbf{w}^*\hat{p}_j(A)\hat{p}_j(A)\mathbf{v}} = \sqrt{\hat{\mathbf{w}}_j^*\hat{\mathbf{v}}_j}, \quad j = 1, \ldots, n-1.$$

The vectors $\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}$ satisfy the three-term recurrence relation (2.3)

$$\beta_j \mathbf{v}_j = (A - \alpha_{j-1})\mathbf{v}_{j-1} - \beta_{j-1}\mathbf{v}_{j-2}, \qquad \text{for } j = 1, \ldots, n-1.$$

Since $\mathbf{w}_j = \bar{\tilde{p}}_j(A^*)\,\mathbf{w}$,

$$\bar{\beta}_j \mathbf{w}_j = (A^* - \bar{\alpha}_{j-1})\mathbf{w}_{j-1} - \bar{\beta}_{j-1}\mathbf{w}_{j-2}, \qquad \text{for } j = 1, \ldots, n-1.$$

The resulting form of the Lanczos algorithm is given as Algorithm 2.3. The matrices $V_n = [\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}]$ and $W_n = [\mathbf{w}_0, \ldots, \mathbf{w}_{n-1}]$ satisfy

$$AV_n = V_n J_n + \hat{\mathbf{v}}_n \mathbf{e}_n^T,$$
$$A^* W_n = W_n J_n^* + \hat{\mathbf{w}}_n \mathbf{e}_n^T,$$

with $\mathbf{e}_n$ the nth vector of the canonical basis, J_n the Jacobi matrix associated with the polynomials $\tilde{p}_0, \ldots, \tilde{p}_{n-1}$,

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

and α_{n-1}, $\hat{\mathbf{v}}_n$, $\hat{\mathbf{w}}_n$ are to be computed at the step n of the Lanczos algorithm[1]. The biorthogonality conditions (2.2) then give

$$W_n^* V_n = I_n,$$
$$W_n^* A V_n = J_n,$$

where I_n is the identity matrix of dimension n. Algorithm 2.3 can be seen as a restriction of A to the Krylov subspace $\mathcal{K}_n(A, \mathbf{v})$ with the subsequent projection orthogonal to $\mathcal{K}_n(A^*, \mathbf{w})$. The reduced operator on $\mathcal{K}_n(A, \mathbf{v})$ then can be expressed via the Jacobi matrix J_n. We say that Lanczos algorithm 2.3 is based on orthonormal polynomials. Obviously, any other scaling of orthogonal polynomials can be used, i.e., the Lanczos algorithm can be based on any sequence of orthogonal polynomials associated to the linear functional (2.1). For further discussion on the Lanczos algorithm see, e.g., [17, Sections 2.4.1 and 2.4.2].

Recall that if $\mathcal{L}$ is quasi-definite on $\mathcal{P}_{n-1}$, then $\beta_j = \sqrt{\mathcal{L}(\hat{p}_j^2)}$ must be different from zero for $j = 1, \ldots, n-1$. Therefore no breakdown can occur in the first $n-1$ steps of the Lanczos algorithm. There is a breakdown at the step n if and only if $\beta_n = 0$. This can happen in two cases:

1. one of the vectors $\hat{\mathbf{v}}_n$ and $\hat{\mathbf{w}}_n$ is the zero vector,
2. $\hat{\mathbf{v}}_n \neq \mathbf{0}$ and $\hat{\mathbf{w}}_n \neq \mathbf{0}$, but $\hat{\mathbf{w}}_n^* \hat{\mathbf{v}}_n = 0$.

In the first case either $\mathcal{K}_n(A, \mathbf{v})$ is A-invariant or $\mathcal{K}_n(A^*, \mathbf{w})$ is A^*-invariant. This is known as *lucky breakdown* (or *benign breakdown*) because the computation of an invariant subspace is often a desirable result; see, e.g., [20, Section 5] and [9, Section 10.5.5]. The second case is known as *serious breakdown*; for an analysis we refer to [22], [14, p. 34], [20, Section 7], and [11, 12]. The previous development is summarized in the following Theorem, cf. also [3, 20].

THEOREM 2.4. *Let $A \in \mathbb{C}^{N\times N}$, $\mathbf{v} \in \mathbb{C}^N$ and $\mathbf{w} \in \mathbb{C}^N$ be the input for the Lanczos algorithm, let $m_k = \mathbf{w}^* A^k \mathbf{v}$, and let Δ_k be the corresponding Hankel determinants (1.1) for $k = 0, 1, \ldots$. There are no breakdowns at the first $n-1$ steps of the Lanczos algorithm if and only if*

$$\prod_{k=0}^{n-1} \Delta_k \neq 0. \tag{2.6}$$

There is a breakdown at the subsequent step n if and only if, in addition to (2.6), $\Delta_n = 0$. In other words, the Lanczos algorithm has a breakdown at the step n if and only if the linear functional (2.1) is quasi-definite on $\mathcal{P}_{n-1}$, but not on $\mathcal{P}_n$.

If the matrix A is Hermitian, $\mathbf{v} = \mathbf{w} \neq 0$, and $d = d(A, \mathbf{v})$ is the grade of $\mathbf{v}$ with respect to A, then the moments of $\mathcal{L}$ defined by (2.1) are real and $\mathcal{L}$ is a *positive-definite linear functional* on $\mathcal{P}_{d-1}$, i.e., the corresponding Hankel determinants Δ_j, $j = 0, \ldots, d-1$, are positive; see [21, Section 2] and the references given there. Obviously, $\Delta_d = 0$. The bilinear form $\mathcal{L}(pq)$ is a discrete inner product on $\mathcal{P}_{d-1}$ and there exists the positive non-decreasing distribution function μ supported on the real axis having finitely many points of increase such that

$$\mathcal{L}(p) = \int_{\mathbb{R}} p(x) \mathrm{d}\mu(x), \qquad \text{for } p \in \mathcal{P}_{2d-1},$$

[1]The coefficient α_{n-1} present in J_n, and the vectors $\hat{\mathbf{v}}_n$ and $\hat{\mathbf{w}}_n$ are well defined even in the case of breakdown at the step n.

which is the Stieltjes representation of the functional $\mathcal{L}$.

3. Gauss quadrature and the Lanczos algorithm. We start this Section by recalling the definition of *matrix function*; see, e.g., [13]. A function f is *defined on the spectrum of the given matrix* A if for every eigenvalue λ_i of A there exist $f^{(j)}(\lambda_i)$ for $j = 0, 1, \dots, s_i - 1$, where s_i is the order of the largest Jordan block of A in which λ_i appears. Let Λ be a Jordan block of A of the size s corresponding to the eigenvalue λ. The matrix function $f(\Lambda)$ is then defined as

$$f(\Lambda) = \begin{bmatrix} f(\lambda) & \frac{f'(\lambda)}{1!} & \frac{f^{(2)}(\lambda)}{2!} & \dots & \frac{f^{(s-1)}(\lambda)}{(s-1)!} \\ 0 & f(\lambda) & \frac{f'(\lambda)}{1!} & \dots & \frac{f^{(s-2)}(\lambda)}{(s-2)!} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \frac{f'(\lambda)}{1!} \\ 0 & \dots & \dots & 0 & f(\lambda) \end{bmatrix}.$$

Denoting

$$A = W \mathrm{diag}(\Lambda_1, \dots, \Lambda_\nu) W^{-1}$$

the Jordan decomposition of A, the *matrix function* $f(A)$ is defined by

$$f(A) = W \mathrm{diag}(f(\Lambda_1), \dots, f(\Lambda_\nu)) W^{-1}.$$

Given a linear functional $\mathcal{L}$ on the space of sufficiently smooth functions, consider the quadrature of the form (see [21, Section 7])

$$\mathcal{L}(f) \approx \sum_{i=1}^{\ell} \sum_{j=0}^{s_i - 1} \omega_{i,j}\, f^{(j)}(\lambda_i), \quad n = s_1 + \dots + s_\ell, \tag{3.1}$$

with $\omega_{i,j}$ the weights, λ_i the nodes, and s_i the multiplicity of the node λ_i. Notice that the number of *different* nodes in (3.1) is equal to ℓ, and ℓ can be less than n. If we count the multiplicities, then the number of nodes is equal to n, that is also the number of weights in (3.1). In order to avoid ambiguity, we refer to (3.1) as the n-weight quadrature, instead of the n-point or n-node quadrature as is usually done. For any choice of (different) nodes λ_i, $i = 1, \dots, \ell$, and their multiplicities s_i, such that $s_1 + \dots + s_\ell = n$, it is possible to achieve that the quadrature (3.1) is exact for any f from $\mathcal{P}_{n-1}$. As shown in the proof of Theorem 7.1 in [21], it is necessary and sufficient to take

$$\omega_{i,j} = \mathcal{L}(h_{i,j}), \tag{3.2}$$

where $h_{i,j}$ are polynomials from $\mathcal{P}_{n-1}$ such that

$$h_{i,j}^{(t)}(\lambda_k) = 1 \quad \text{for } \lambda_k = \lambda_i \text{ and } t = j,$$
$$h_{i,j}^{(t)}(\lambda_k) = 0 \quad \text{for } \lambda_k \neq \lambda_i \text{ or } t \neq j,$$

with $k = 1, 2, \dots, \ell$, and $t = 0, 1, \dots, s_i - 1$. In this case we say that the quadrature (3.1) is interpolatory, since it can be obtained by applying the linear functional $\mathcal{L}$ to the generalized (Hermite) interpolating polynomial for the function f at the nodes λ_i of the multiplicities s_i.

We refer to (3.1) as the (complex) Gauss quadrature if and only if the following three properties are satisfied.

- G1: n-weight Gauss quadrature attains the maximal algebraic degree of exactness $2n-1$, i.e., it is exact for all polynomials of degree at most $2n-1$.
- G2: n-weight Gauss quadrature is well-defined and it is unique. Moreover, Gauss quadratures with a smaller number of weights also exist and they are unique.
- G3: Gauss quadrature of a function f can be written as the quadratic form $m_0\, \mathbf{e}_1^T f(J_n)\mathbf{e}_1$, where J_n is the complex 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 will further use the word "complex" in the name of the quadrature only when it is necessary to emphasize the difference with respect to the standard Gauss quadrature. The following theorem is proved in [21, Section 7].

THEOREM 3.1. *Let $\mathcal{L}$ be a linear functional on $\mathcal{P}$. There exists the n-weight quadrature (3.1) having properties G1, G2 and G3 if and only if $\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$.*

The nodes λ_i, $i = 1, \ldots, \ell$, of the n-weight Gauss quadrature, and their multiplicities s_i, $s_1 + \cdots + s_\ell = n$, are such that

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

is the nth degree monic orthogonal polynomial with respect to $\mathcal{L}$. The weights of the n-weight Gauss quadrature are given by (3.2).

If the quasi-definite linear functional on $\mathcal{P}_n$ is given by (2.1), then the associated Jacobi matrix can be constructed by performing n steps of the Algorithm 2.3; see Section 2. Keeping in mind the property G3, for this kind of linear functionals we can say that the Lanczos algorithm is a matrix formulation of the Gauss quadrature.

Moreover, we can 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 approximating $\mathcal{L}$, 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

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

Indeed, let $A \in \mathbb{C}^{2n\times 2n}$ and $\mathbf{w} \in \mathbb{C}^{2n}$ be such that the matrix

$$B = [\mathbf{w}, A^*\mathbf{w}, \ldots, (A^*)^{2n-1}\mathbf{w}]$$

is nonsingular, and construct the vector $\mathbf{v}$ as the solution of the linear system

$$B^*\mathbf{v} = \mathbf{m}, \quad \mathbf{m} = [m_0, m_1, \ldots, m_{2n-1}]^T.$$

Then the first $2n$ moments of $\mathcal{L}$ and the first $2n$ moments of the functional $\tilde{\mathcal{L}}(f) = \mathbf{w}^* f(A)\mathbf{v}$ are equal. This means that the n-weight Gauss quadrature for $\mathcal{L}$ can be identified with $m_0\mathbf{e}_1^T f(J_n)\mathbf{e}_1$, where J_n is the Jacobi matrix obtained in the step n of the Algorithm 2.3 with the input A, $\mathbf{v}$ and $\mathbf{w}$.

Notice that the matrix J_n from the previous two paragraphs (that requires quasi-definiteness of $\mathcal{L}$ on $\mathcal{P}_{n-1}$) is well defined even in the case of the breakdown at the step n of the Lanczos algorithm. If $\mathcal{L}$ is not quasi-definite on $\mathcal{P}_n$, then, however, the quadrature rule $\mathcal{L}(f) \approx m_0\mathbf{e}_1^T f(J_n)\mathbf{e}_1$ is not the Gauss quadrature since its degree of exactness is larger then $2n-1$, i.e.,

$$\mathcal{L}(x^k) = m_0\mathbf{e}_1^T J_n^k \mathbf{e}_1, \ \ k = 0, \ldots, j,$$

where $j \geq 2n$; see [21, Sections 7 and 8].

4. Jordan decomposition of complex Jacobi matrices. Let J_n be an arbitrary $n \times n$ complex Jacobi matrix. Then there exists a linear functional $\mathcal{L}$ quasi-definite on $\mathcal{P}_n$ such that J_n contains the coefficients from the three-term recurrence relation for orthonormal polynomials $\tilde{p}_j$, $j = 0, \dots, n$, associated with $\mathcal{L}$. J_n is a non-derogatory matrix (see, e.g., [21, Section 4]), i.e., it has ℓ distinct eigenvalues $\lambda_1, \dots, \lambda_\ell$, all having the geometric multiplicity 1. We write its Jordan decomposition as

$$J_n = W \mathrm{diag}(\Lambda_1, \dots, \Lambda_\ell) W^{-1}, \tag{4.1}$$

where Λ_i is the Jordan block of dimension s_i associated with the eigenvalue λ_i, $i = 1, \dots, \ell$. For any $t = 1, \dots, n$ there is exactly one integer i between 1 and ℓ, and exactly one integer j between 0 and $s_i - 1$, such that $t = s_1 + \ldots + s_{i-1} + j + 1$ (here, for $i = 0$, $s_0 \equiv 0$). In other words, fixed t uniquely determines i and j, and vice versa, fixed i and j uniquely determine t. The t-th column $\mathbf{w}_{t(i,j)}$ of W can be written as (see, e.g., [21, Proposition 4.4])

$$\mathbf{w}_{t(i,j)} = \frac{1}{j!} \begin{bmatrix} \mathbf{0}_j \\ \tilde{p}_j^{(j)}(\lambda_i) \\ \vdots \\ \tilde{p}_{n-1}^{(j)}(\lambda_i) \end{bmatrix}, \tag{4.2}$$

where $\mathbf{0}_j$ is the zero vector of length j. The next theorem gives the explicit formula for the rows of W^{-1}.

Theorem 4.1. *Let $J_n = W \mathrm{diag}(\Lambda_1, \dots, \Lambda_\ell) W^{-1}$ be the Jordan decomposition of an $n \times n$ complex Jacobi matrix J_n. Let $\mathcal{L}$ be the quasi-definite linear functional on $\mathcal{P}_n$ such that J_n contains the coefficients from the three-term recurrence relation for the orthonormal polynomials $\tilde{p}_0, \dots, \tilde{p}_n$ with respect to $\mathcal{L}$, and let $\sum_{i=1}^{\ell} \sum_{j=0}^{s_i-1} \omega_{i,j}\, f^{(j)}(\lambda_i)$ be the Gauss quadrature for $\mathcal{L}$ defined by* (3.1) *and* (3.2)*. Then the r-th row $\mathbf{v}_{r(i,j)}^T$ of W^{-1},*

$$\mathbf{v}_{r(i,j)}^T = \mathbf{e}_{r(i,j)}^T W^{-1}, \quad r = s_1 + \cdots + s_{i-1} + j + 1 \quad (s_0 \equiv 0 \textit{ for } i = 1),$$

has the following representation

$$\mathbf{v}_{r(i,j)} = \sum_{\nu=j}^{s_i-1} \nu!\, \omega_{i,\nu}\, \mathbf{w}_{t(i,\nu-j)}, \tag{4.3}$$

with $\mathbf{w}_{t(i,\nu-j)}$ defined by (4.2).

Proof. Let V be the $n \times n$ matrix with the rows $\mathbf{v}_{r(i,j)}$, $r = 1, \dots, n$, given by (4.3). We will show that $WV = I_n$, i.e., $V = W^{-1}$. Denote the k-th row of W by $\mathbf{a}_k^T$, and the m-th column of V by $\mathbf{b}_m$ and prove that

$$\mathbf{a}_k^T \mathbf{b}_m = \mathcal{L}(\tilde{p}_{k-1} \tilde{p}_{m-1}).$$

By (4.2) the q-th element of $\mathbf{a}_k$ is

$$a_{k,q} = \frac{\tilde{p}_{k-1}^{(j)}(\lambda_i)}{j!}, \quad q = s_0 + s_1 + \ldots + s_{i-1} + j + 1,$$

where for $k-1<j$ we have $\tilde{p}_{k-1}^{(j)}(\lambda_i)=0$. Using (4.3), the q-th element of $\mathbf{b}_m$ is

$$b_{m,q}=\sum_{\nu=j}^{s_i-1}\nu!\,\omega_{i,\nu}\,\frac{\tilde{p}_{m-1}^{(\nu-j)}(\lambda_i)}{(\nu-j)!}=j!\sum_{\nu=j}^{s_i-1}\binom{\nu}{j}\omega_{i,\nu}\,\tilde{p}_{m-1}^{(\nu-j)}(\lambda_i).$$

Thus we get by rearranging the order of summations

$$\begin{aligned}\sum_{q=1}^{n}a_{k,q}b_{m,q}&=\sum_{q=1}^{n}\sum_{\nu=j}^{s_i-1}\binom{\nu}{j}\omega_{i,\nu}\,\tilde{p}_{m-1}^{(\nu-j)}(\lambda_i)\tilde{p}_{k-1}^{(j)}(\lambda_i)\\&=\sum_{i=1}^{\ell}\sum_{j=0}^{s_i-1}\omega_{i,j}\sum_{u=0}^{j}\binom{j}{u}\tilde{p}_{m-1}^{(j-u)}(\lambda_i)\tilde{p}_{k-1}^{(u)}(\lambda_i)\\&=\sum_{i=1}^{\ell}\sum_{j=0}^{s_i-1}\omega_{i,j}(\tilde{p}_{m-1}\tilde{p}_{k-1})^{(j)}(\lambda_i)=\mathcal{L}(\tilde{p}_{k-1}\tilde{p}_{m-1}),\end{aligned}$$

which gives the result. □

REMARK 4.2. *The fact that a Jacobi matrix J_n is symmetric is associated with the requirement $WV=I_n$ and the orthogonal polynomials $\tilde{p}_j$, $j=0,\ldots,n$ being orthonormal. The previous development can be easily modified for the Jordan decomposition $T_n=W\mathrm{diag}(\Lambda_1,\ldots,\Lambda_\ell)W^{-1}$ of an arbitrary irreducible tridiagonal matrix T_n. The representation (4.2) of the columns of W will then use the orthogonal polynomials p_j satisfying the three-term recurrence relation with the coefficients given by T_n (see, e.g., [21, Proposition 4.4]),*

$$\mathbf{w}_{t(i,j)}=\frac{1}{j!}\begin{bmatrix}\mathbf{0}_j\\p_j^{(j)}(\lambda_i)\\\vdots\\p_{n-1}^{(j)}(\lambda_i)\end{bmatrix}.\tag{4.4}$$

The matrix V with the rows defined by (4.3) satisfies

$$WV=diag(\mathcal{L}(p_0^2),\ldots,\mathcal{L}(p_{n-1}^2)),$$

i.e.,

$$W^{-1}=V\,diag(1/\mathcal{L}(p_0^2),\ldots,1/\mathcal{L}(p_{n-1}^2)).$$

The rows of W^{-1} can then be written as

$$\mathbf{v}_{r(i,j)}=\sum_{\nu=j}^{s_i-1}\nu!\,\omega_{i,\nu}\,\tilde{\mathbf{w}}_{t(i,\nu-j)},\tag{4.5}$$

where

$$\tilde{\mathbf{w}}_{t(i,j)}=\frac{1}{j!}\begin{bmatrix}\mathbf{0}_j\\p_j^{(j)}(\lambda_i)/\mathcal{L}(p_j^2)\\\vdots\\p_{n-1}^{(j)}(\lambda_i)/\mathcal{L}(p_{n-1}^2)\end{bmatrix}.\tag{4.6}$$

5. Gauss quadrature for a linear functional with real moments. Let us focus now on the n-weight Gauss quadrature $\mathcal{G}_n$ for approximating a real-valued linear functional $\mathcal{L}$ on the space of sufficiently smooth real-valued functions. At first glance, the idea of approximating such a functional by the quadrature with complex nodes and weights does not seem attractive. We will show that the value of $\mathcal{G}_n(f)$, for suitable f, is always a real number.

THEOREM 5.1. *Let $\mathcal{L}$ be a quasi-definite linear functional on $\mathcal{P}_n$ whose moments $m_0, \dots, m_{2n-1}$ are real, and let $\mathcal{G}_n$ be the 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. *The nodes λ_i, $i = 1, \dots, \ell$ are real or appear in complex conjugate pairs, i.e., for any $\lambda_i \notin \mathbb{R}$ with multiplicity s_i there is a node $\lambda_m = \overline{\lambda}_i$ with the same multiplicity.*
2. *For any $\lambda_i \in \mathbb{R}$ we have $\omega_{i,j} \in \mathbb{R}$, $j = 0, \dots, s_i - 1$. If $\lambda_i \notin \mathbb{R}$ and $\lambda_m = \overline{\lambda}_i$, then $\omega_{m,j} = \overline{\omega}_{i,j}$ for $j = 0, \dots, s_i - 1$.*
3. *If f is a real-valued function satisfying $f^{(j)}(\overline{\lambda}_i) = \overline{f^{(j)}(\lambda_i)}$ for $i = 1, \dots, \ell$ and $j = 0, \dots, s_i - 1$, then $\mathcal{G}_n(f)$ is a real number.*

Proof. The monic orthogonal polynomials $\pi_0, \pi_1, \dots, \pi_n$ associated with $\mathcal{L}$ satisfy

$$\pi_j(x) = (x - \alpha_{j-1})\pi_{j-1}(x) - \eta_{j-1}\pi_{j-2}(x), \quad j = 1, 2, \dots, n,$$

with $\alpha_0 = m_1/m_0, \pi_{-1}(x) = 0$, $\pi_0(x) = 1$, and

$$\alpha_{j-1} = \frac{\mathcal{L}(x\pi_{j-1}^2)}{\mathcal{L}(\pi_{j-1}^2)}, \quad \eta_{j-1} = \frac{\mathcal{L}(\pi_{j-1}^2)}{\mathcal{L}(\pi_{j-2}^2)}, \quad j = 2, \dots, n\,.$$

The moments of $\mathcal{L}$ are real, which implies that $\alpha_{j-1}, \eta_{j-1} \in \mathbb{R}$ for $j = 2, \dots, n$, and the polynomials π_j, $j = 0, \dots, n$ have (only) real coefficients. Thus we proved the first statement of the Theorem. The tridiagonal matrix T_n associated with $\pi_0, \dots, \pi_n$ is a real matrix. Under the assumptions made on f, the matrix $f(B)$ is real for any real matrix B; see [13, Remark 1.9]. Hence $\mathcal{G}_n(f)$ is a real number since

$$\mathcal{G}_n(f) = m_0 \mathbf{e}_1^T f(J_n)\mathbf{e}_1 = m_0 \mathbf{e}_1^T f(T_n)\mathbf{e}_1;$$

see property G3 and Theorem 1.4.

We will prove the statement 2 by induction on j, using the Jordan decomposition $T_n = W \mathrm{diag}(\Lambda_1, \dots, \Lambda_\ell) W^{-1}$ and expressions (4.4), (4.5), and (4.6). If λ_i is not real, then there exists the eigenvalue $\lambda_m = \overline{\lambda}_i$, with $s_m = s_i$. Since $\pi_k(\bar{x}) = \overline{\pi_k(x)}$ for $k = 0, \dots, n$, then

$$\mathbf{w}_{t(i,j)} = \overline{\mathbf{w}_{u(m,j)}}, \quad \tilde{\mathbf{w}}_{t(i,j)} = \overline{\tilde{\mathbf{w}}_{u(m,j)}}, \quad j = 0, \dots, s_i - 1.$$

Fix $j = s_i - 1 = s_m - 1$ as the base case of the inductive proof. Then, expression (4.5) gives

$$(\mathbf{v}_{r(i,s_i-1)})^T = (s_i - 1)!\, \omega_{i,s_i-1} (\tilde{\mathbf{w}}_{t(i,0)})^T,$$

$$(\mathbf{v}_{q(m,s_m-1)})^T = (s_i - 1)!\, \omega_{m,s_m-1} (\tilde{\mathbf{w}}_{t(i,0)})^*.$$

Using $(\mathbf{v}_{r(i,s_i-1)})^T \mathbf{w}_{r(i,s_i-1)} = 1$ and $(\mathbf{v}_{q(m,s_m-1)})^T \overline{\mathbf{w}_{r(i,s_i-1)}} = 1$ with the two previous equations, it follows that

$$\frac{1}{\omega_{i,s_i-1}} = (s_i-1)!\,(\tilde{\mathbf{w}}_{t(i,0)})^T \mathbf{w}_{r(i,s_i-1)} \quad \text{and} \quad \frac{1}{\omega_{m,s_m-1}} = (s_i-1)!\,\overline{(\tilde{\mathbf{w}}_{t(i,0)})^T \mathbf{w}_{r(i,s_i-1)}}\,.$$

Hence, $\omega_{i,s_i-1} = \overline{\omega}_{m,s_m-1}$, which finishes the initial step. Let us fix j between 0 and s_i-2 and let $\omega_{i,k} = \overline{\omega}_{m,k}$, $k = j+1, \ldots, s_i-1$, be the inductive assumptions. Then, $(\mathbf{v}_{t(i,j)})^T \mathbf{w}_{t(i,j)} = 1$ and (4.5) give

$$\sum_{\nu=j}^{s_i-1} \nu!\,\omega_{i,\nu}\,(\tilde{\mathbf{w}}_{r(i,\nu-j)})^T \mathbf{w}_{t(i,j)} = 1.$$

The first summand on the left-hand side of the previous equation can be written as

$$\begin{aligned} j!\,\omega_{i,j}\,(\tilde{\mathbf{w}}_{r(i,0)})^T \mathbf{w}_{t(i,j)} &= 1 - \sum_{\nu=j+1}^{s_i-1} \nu!\,\omega_{i,\nu}\,(\tilde{\mathbf{w}}_{r(i,\nu-j)})^T \mathbf{w}_{t(i,j)} \\ &= 1 - \sum_{\nu=j+1}^{s_i-1} \nu!\,\overline{\omega}_{m,\nu}\,\overline{(\tilde{\mathbf{w}}_{q(m,\nu-j)})^T}\ \overline{\mathbf{w}_{u(m,j)}} \\ &= j!\,\overline{\omega_{m,j}\,(\tilde{\mathbf{w}}_{q(m,0)})^T \mathbf{w}_{u(m,j)}} \\ &= j!\,\overline{\omega}_{m,j}\,(\tilde{\mathbf{w}}_{r(i,0)})^T \mathbf{w}_{t(i,j)}. \end{aligned}$$

Therefore, $\omega_{i,j} = \overline{\omega}_{m,j}$ for $j = 0, \ldots, s_i-1$.

If $\lambda_i \in \mathbb{R}$, then an analogous induction gives $\omega_{i,j} \in \mathbb{R}$, $j = 0, \ldots, s_i-1$. Notice that, in this case, the vectors $\mathbf{w}_{t(i,j)}$ and $\tilde{\mathbf{w}}_{t(i,j)}$ are real. □

Among all tridiagonal matrices determined by the first $2n$ real moments of the given linear functional $\mathcal{L}$ quasi-definite on $\mathcal{P}_n$, there must be a real matrix (see Section 1). By (1.5) we conclude that all tridiagonal matrices determined by real moments have real numbers on the main diagonal. By (1.6), the elements at the super-diagonal of the corresponding Jacobi matrix (that is complex symmetric) are either real or pure imaginary. They are all real if and only if the linear functional $\mathcal{L}$ is positive definite on $\mathcal{P}_n$; see, e.g., [19, Theorem 2.14].

We now apply the previous discussion to the Lanczos algorithm with a real input. Obviously, the moments of the linear functional $\mathcal{L}$ defined by (2.1) are real. The output after n steps of the Lanczos algorithm is real if and only if the algorithm is based on orthogonal polynomials satisfying the three-term recurrence relation with real coefficients. Since Algorithm 2.3 is based on orthonormal polynomials, it cannot result in a real output after n steps unless the functional (2.1) is positive definite on $\mathcal{P}_n$. The output after n steps of the Lanczos algorithm is real providing that the algorithm is based on monic orthogonal polynomials. However, in this case there is no scaling of the vectors $\hat{\mathbf{v}}_j$ and $\hat{\mathbf{w}}_j$. If the scaling of the vectors $\hat{\mathbf{v}}_j, \hat{\mathbf{w}}_j$ is required (for any reason), then one can use the following orthogonal polynomials; cf. [10, Section 2]. The polynomials $p_0 = \tilde{p}_0, \ldots, p_{j-1} = \tilde{p}_{j-1}$ are constructed by Algorithm 2.2 as long as they have real coefficients, i.e., as long as $\mathcal{L}(\hat{p}_k^2)$, $k = 0, \ldots, j-1$, is positive. When $\mathcal{L}(\hat{p}_j^2)$ is negative, then we scale $\hat{p}_j$ in the following way:

$$\delta_j = \sqrt{|\mathcal{L}(\hat{p}_j^2)|}, \qquad p_j = \frac{\hat{p}_j}{\delta_j}.$$

Algorithm 5.2 (Lanczos algorithm in the real number setting).
Input: real matrix A, two real vectors $\mathbf{v}, \mathbf{w}$ such that $\mathbf{w}^*\mathbf{v} \neq 0$.
Output: vectors $\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}$ that span $\mathcal{K}_n(A, \mathbf{v})$ and vectors $\mathbf{w}_0, \ldots, \mathbf{w}_{n-1}$ that span $\mathcal{K}_n(A^*, \mathbf{w})$, satisfying the biorthogonality conditions (2.2).

Initialize: $\mathbf{v}_{-1} = \mathbf{w}_{-1} = 0$, $\gamma_0 = 0$, $\hat{s} = 1$, $s = 1$,
$\mathbf{v}_0 = \mathbf{v}/||\mathbf{v}||$, $\mathbf{w}_0 = \mathbf{w}/(\mathbf{w}^*\mathbf{v}_0)$.
For $j = 1, 2, \ldots, n$
$\alpha_{j-1} = s \cdot \mathbf{w}_{j-1}^* A \mathbf{v}_{j-1}$,
$\hat{\mathbf{v}}_j = A\mathbf{v}_{j-1} - \alpha_{j-1}\mathbf{v}_{j-1} - \gamma_{j-1}\mathbf{v}_{j-2}$,
$\hat{\mathbf{w}}_j = A^*\mathbf{w}_{j-1} - \alpha_{j-1}\mathbf{w}_{j-1} - \gamma_{j-1}\mathbf{w}_{j-2}$,
$s = sign\,(\hat{\mathbf{w}}_j^*\hat{\mathbf{v}}_j)$,
if $s = 0$ *then stop,*
$\delta_j = \sqrt{|\hat{\mathbf{w}}_j^*\hat{\mathbf{v}}_j|}$,
$\gamma_j = s \cdot \hat{s} \cdot \delta_j$,
$\hat{s} = s$,
$\mathbf{v}_j = \hat{\mathbf{v}}_j/\delta_j$,
$\mathbf{w}_j = \hat{\mathbf{w}}_j/\delta_j$,
end.

Thus we get the sequence of orthogonal polynomials such that $\mathcal{L}(p_j^2)$ is either 1 or -1. The other coefficients from the three-term recurrence relation are also real. They are given by

$$\gamma_j = \frac{\mathcal{L}(xp_{j-1}p_j)}{\mathcal{L}(p_{j-1}^2)} = \frac{\mathcal{L}(p_j^2)}{\mathcal{L}(p_{j-1}^2)}\delta_j = \begin{cases} \delta_j, & \text{if} \quad \mathcal{L}(p_{j-1}^2)\cdot\mathcal{L}(p_j^2) = 1 \\ -\delta_j, & \text{if} \quad \mathcal{L}(p_{j-1}^2)\cdot\mathcal{L}(p_j^2) = -1, \end{cases}$$

$$\alpha_j = \frac{\mathcal{L}(xp_j^2)}{\mathcal{L}(p_j^2)} = \begin{cases} \mathcal{L}(xp_j^2), & \text{if} \quad \mathcal{L}(p_j^2) = 1 \\ -\mathcal{L}(xp_j^2), & \text{if} \quad \mathcal{L}(p_j^2) = -1. \end{cases}$$

The resulting form of the Lanczos algorithm involving only real number computations is given as Algorithm 5.2. The tridiagonal matrix $T_n = W_n^* A V_n$ obtained by the first n iterations of the algorithm has sub- and super-diagonal elements such that $\delta_j = \gamma_j$ or $\delta_j = -\gamma_j$, for $j = 1, \ldots, n-1$.

6. Conclusion. The paper presents the Lanczos algorithm as a matrix representation of the complex Gauss quadrature. It justifies the approach from [21] where we argue that the complex Gauss quadrature must inherit the properties G1, G2 and G3 of the Gauss quadrature for the positive definite functionals. The weights $\omega_{i,j}$ from the Gauss quadrature (3.1) appear in the representation (4.3) of the rows of W^{-1} from the Jordan decomposition (4.1) of the corresponding complex Jacobi matrix. When the moments of the quasi-definite linear functional approximated by the Gauss quadrature $\mathcal{G}_n$ are real, then the non-real nodes and weights of $\mathcal{G}_n$ come in the conjugate pairs. Therefore the value of $\mathcal{G}_n(f)$ is a real number whenever the real-valued function f satisfies $f^{(j)}(\bar{\lambda}_i) = \overline{f^{(j)}(\lambda_i)}$ for $i = 1, \dots, \ell$ and $j = 0, \dots, s_i - 1$. This property is linked with the fact that if the input is real, then the Lanczos algorithm with an appropriate scaling can be performed in the real number setting.

If the linear functional $\mathcal{L}$ is not quasi-definite on $\mathcal{P}_n$, then the maximal algebraic degree of exactness of the n-weight quadrature (3.1) is not a priori given. The associated questions, which are related to the existence and uniqueness of the nth degree orthogonal polynomial with respect to $\mathcal{L}$, will be considered in a further work.

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