Shifted Lanczos method for quadratic forms with Hermitian matrix resolvents

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Abstract

Quadratic forms of Hermitian matrix resolvents involve the solutions of shifted linear systems. Efficient solutions use the shift-invariance property of Krylov subspaces. The Hermitian Lanczos method reduces a given vector and matrix to a Jacobi matrix (a real symmetric tridiagonal matrix with positive super and sub-diagonal entries) and approximates the quadratic form with the Jacobi matrix. This study develops a shifted Lanczos method that deals directly with the Hermitian matrix resolvent to extend the scope of problems that the Lanczos method can solve. We derive a matrix representation of a linear operator that approximates the resolvent by solving a Vorobyev moment problem associated with the shifted Lanczos method. We show that an entry of the Jacobi matrix resolvent can approximate the quadratic form. We show the moment-matching property of the shifted Lanczos method and give a sufficient condition such that the method does not break down. Numerical experiments on matrices drawn from real-world applications compare the proposed method with previous methods and show that the proposed method outperforms a well-established method in solving some problems.

1 Introduction

Consider the computation of \( m \) quadratic forms

\[
v^H(z_i I - A)^{-1} v, \quad i = 1, 2, \ldots, m, \tag{1.1}\]

where \( v^H \) denotes the complex conjugate transpose of a vector \( v \in \mathbb{C}^n \), \( A \in \mathbb{C}^{n \times n} \) is a Hermitian matrix and \( z_i \in \mathbb{C} \). Here, \( z_i I - A \) is assumed to be invertible. This kind of problem arises in chemistry and physics (Liesen & Strakoš, 2013, Section 3.9), eigensolvers using complex moments (Sakurai & Tadano, 2007), the stochastic estimation of the number of eigenvalues (Maeda et al., 2015), samplers for determinantal point processes (Li et al., 2016, and references therein) and the approximation of Markov chains in Bayesian sampling (Johndrow et al., 2017). An extension of the present single-vector case \( v \in \mathbb{R}^n \) in (1.1) for real \( A \in \mathbb{R}^{n \times n} \) to the multiple-vector case \( v_1, v_2, \ldots, v_\ell \in \mathbb{R}^n \), namely,

\[
V^\top (z_i I - A)^{-1} V, \quad V = [v_1, v_2, \ldots, v_\ell] \in \mathbb{R}^{n \times \ell}, \quad i = 1, 2, \ldots, m
\]

can be reduced to the solutions of bilinear forms \( v_p^\top (z_i I - A) v_q, \quad p, q = 1, 2, \ldots, \ell, \) where \( v_p \) is the \( p \)th column of \( V \). The bilinear form \( v_p (z_i I - A)^{-1} v_q \) can be reduced to the quadratic form

\[
v_p (z_i I - A)^{-1} v_q = \frac{1}{4} [s^\top (z_i I - A)^{-1} s - t^\top (z_i I - A)^{-1} t]
\]

where \( s \) and \( t \) are the solutions of the shifted linear systems.

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where \( s = v_p + v_q \) and \( t = v_p - v_q \) (cf. Golub & Meurant 2010, p. 114). This kind of problem arises in the analysis of dynamical systems (Bai & Golub 2002).

A straightforward approach to the quadratic form (1.1) is to solve the shifted linear systems

\[
(zI - A)x^{(i)} = v
\]

and compute \( v^H x^{(i)} \) for \( i = 1, 2, \ldots, m \). The development of efficient solutions for solving shifted linear systems (1.2) with real symmetric \( A \) has been ongoing for two decades; they include shifted Krylov subspace methods such as variants of the conjugate orthogonal conjugate gradient (COCG) method (van der Vorst & Melissen 1990), the quasi-minimal residual (QMR) method (Freund & Nachtigal 1991; Freund 1992) and the conjugate orthogonal conjugate residual (COCR) method (Sogabe & Zhang 2007), proposed by Takayama et al. (2006), Sogabe et al. (2008) and Sogabe & Zhang (2011), respectively. These methods use the shift-invariance property of the Krylov subspace \( K_k(zI - A, v) = K_k(A, v) \), where \( K_k(A, v) = \text{span}\{v_1, Av_1, \ldots, A^{k-1}v_1\} \). Hence, a basis of the Krylov subspace is formed by using a real symmetric matrix \( A \) instead of a shifted matrix \( zI - A \). Thus, they determine an iterate for a seed linear system and then associated iterates for shifted linear systems by taking the iterative residual vectors of the shifted linear systems to be collinear to that of the seed linear system. These methods may suffer from breakdown, i.e. division by zero, although this happens very rarely in practice. Extensions of the MINRES method (Paige & Saunders 1975) to the shifted linear system (1.2) work with Hermitian \( A \) (Gu & Liu 2013; Seito et al. 2019). The MINRES-based approaches do not break down for nonsingular \( zI - A \) and use only real arithmetic for the matrix–vector product for real \( A \).

The biconjugate gradient (BiCG) method does not exploit the symmetry of a coefficient matrix and requires two matrix–vector products per iteration for non-Hermitian matrices (Strakoš & Tichý 2011), whereas the shifted COCG, COCR and MINRES methods require one matrix–vector product per iteration for (1.2).

In this study, we focus on computing the quadratic form (1.1) without directly solving the shifted linear systems (1.2). The key feature of our approach is the development of a shifted Lanczos method. The Hermitian Lanczos method projects an original model represented by \( A \) and \( v \) to a lower-dimensional model and matches the lowest-order moments of the original model with those of the reduced model, whereas the shifted Lanczos method retains such properties of the Hermitian Lanczos method. To derive the method, the Vorobyev moment problem (Vorobyev 1965; Brezinski 1996; Strakoš 2009; Liesen & Strakoš 2013) is useful. The Vorobyev moment problem gives a matrix representation of a linear operator that represents the reduced model to approximate the resolvent \((zI - A)^{-1}\). We show that the \((1, 1)\) entry of the Jacobi matrix resolvent can approximate the quadratic form (1.1) with eight additional operations to the Lanczos method for each shift by using a recursive formula devised by Golub & Meurant (2010). Moreover, we give a sufficient condition such that the proposed method does not break down. To the best of the author’s knowledge, this study is the first of its kind to investigate the effectiveness of the Lanczos method for directly approximating the quadratic form of a Hermitian matrix resolvent.

The outline of this paper is as follows. In Section 2 we review the Lanczos method and its moment-matching property. In Section 3 we describe a shifted Lanczos method for computing the quadratic forms (1.1), show its moment-matching property and implementation, discuss related methods, and give a sufficient breakdown-free condition. In Section 4 we present the results of numerical experiments, comparing the shifted Lanczos method with previous methods, and provide an error estimate for the shifted Lanczos method. In Section 5 we conclude the paper.
2 Lanczos method

Consider the application of the Lanczos method (Lanczos, 1952) to $A$ to approximate the resolvent $(zI - A)^{-1}$. For convenience, we omit subscript $i$ of $z_i$. An algorithm for the Lanczos method is given as Algorithm 2.1.

**Algorithm 2.1 Lanczos method**

| Input: $A \in \mathbb{C}^{n \times n}$, $v \in \mathbb{C}^n$, $z_i \in \mathbb{C}$, $i = 1, 2, \ldots, m$ |
| Output: $v_1 = v/\|v\|$, $u = Av_1$, $\alpha_1 = u^Hv_1$ |
| 1: $v_1 = v/\|v\|$, $u = Av_1$, $\alpha_1 = u^Hv_1$ |
| 2: for $k = 1, 2, \ldots$ do |
| 3: $u = u - \alpha_k v_k$, $\beta_k = \|u\|$ |
| 4: if $\beta_k = 0$ then break |
| 5: $v_{k+1} = (\beta_k)^{-1}u$, $u = Av_{k+1} - \beta_k v_k$, $\alpha_{k+1} = u^Hv_{k+1}$ |
| 6: end for |

Here, $\| \cdot \|$ denotes the Euclidean norm. Denote the Lanczos decomposition of $A$ by

$$AV_k = V_{k+1}T_{k+1,k}, \quad (2.1)$$

where the columns of $V_k = [v_1, v_2, \ldots, v_k]$ form an orthonormal basis of the Krylov subspace $K_k(A, v_1) = \text{span}\{v_1, Av_1, \ldots, A^{k-1}v_1\}$ and $T_{k+1,k}$ is the Jacobi matrix (real symmetric tridiagonal matrix with positive super and sub-diagonal entries)

$$T_{k+1,k} = \begin{bmatrix} \alpha_1 & \beta_1 & 0 \\ \beta_1 & \alpha_2 & \beta_2 \\ & \ddots & \ddots \\ & & \beta_{k-1} & \beta_k \\ 0 & & & \alpha_k \end{bmatrix} \in \mathbb{C}^{(k+1)\times k},$$

where $e_i = [0, 0, \ldots, 0, 1, 0, \ldots, 0] \in \mathbb{R}^k$ is the $i$th standard basis vector. Then $V_k^H AV_k = T_{k,k}$ holds.

2.1 Hamburger moment problem

The Lanczos method projects the original model given by a Hermitian matrix $A$ and an initial vector $v$ to a lower-dimensional model given by $T_{k,k}$ and $e_1$, matching the lowest-order moments of the original model and reduced model; i.e. it approximates a given matrix $A$ via moment matching. A thorough derivation of the moment-matching property (2.6) presented below is given in Liesen & Strakš (2013, Chapter 3). Given a sequence of scalars $\xi_i$, $i = 0, 1, 2, \ldots, 2k - 1$, the problem of finding a non-decreasing real distribution function $w^{(k)}(\lambda)$, $\lambda \in \mathbb{R}$, with $k$ points of increase such that the Riemann–Stieltjes integral is equal to the given sequence of scalars

$$\int_{-\infty}^{\infty} \lambda^i dw^{(k)}(\lambda) = \xi_i, \quad i = 0, 1, \ldots, 2k - 1, \quad (2.2)$$

is called the Hamburger moment problem (Hamburger, 1919, 1920a,b, 1921). The left-hand side of (2.3) is called the $i$th moment with respect to the distribution function $w^{(k)}(\lambda)$. Set another moment as

$$\int_{-\infty}^{\infty} \lambda^i dw(\lambda), \quad i = 0, 1, 2, \ldots, 2k - 1, \quad (2.3)$$
and the distribution function with \( n \) points of increase to

\[
w(\lambda) = \begin{cases} 
0, & \lambda < \lambda_1, \\
\sum_{j=1}^{i-1} w_j, & \lambda_i \leq \lambda < \lambda_{i+1}, \quad i = 1, 2, \ldots, n - 1, \\
\sum_{j=1}^{n} w_j = 1, & \lambda_n \leq \lambda 
\end{cases}
\]  

(2.4)

associated with weights \( w_j = (\mathbf{v}^H \mathbf{u}_j)^2 / \| \mathbf{v} \|^2, \ j = 1, 2, \ldots, n \), where \( \lambda_1 < \lambda_2 < \cdots < \lambda_n \) are the eigenvalues of \( A \) and \( \mathbf{u}_i, \ i = 1, 2, \ldots, n \), are the corresponding eigenvectors. Here, for clarity of exposition, we assume that the eigenvalues of \( A \) are distinct without loss of generality. Then we can express the moment \( \mathbf{m}_k \) as the Gauss–Christoffel quadrature and the quadratic form

\[
\int_{-\infty}^{\infty} \lambda^i d\lambda(w) = \sum_{i=1}^{n} w_i \{ \lambda_i \}^i = \mathbf{v}^H A^i \mathbf{v}, \quad \lambda = 0, 1, 2, \ldots.
\]

Thus, the solution of (2.2) is given by

\[
w^{(k)}(\lambda) = \begin{cases} 
0, & \lambda < \lambda_1^{(k)}, \\
\sum_{j=1}^{i-1} w_{j}^{(k)}, & \lambda_i^{(k)} \leq \lambda < \lambda_{i+1}^{(k)}, \quad i = 1, 2, \ldots, k - 1, \\
\sum_{j=1}^{k} w_{j}^{(k)} = 1, & \lambda_k^{(k)} \leq \lambda 
\end{cases}
\]

(2.5)

associated with weights \( w_{j}^{(k)} = (\mathbf{e}_1^T \mathbf{u}_j^{(k)})^2, \ j = 1, 2, \ldots, k \), where \( \lambda_1^{(k)} < \lambda_2^{(k)} < \cdots < \lambda_k^{(k)} \) are the eigenvalues of \( T_{k,k} \) and \( \mathbf{u}_j^{(k)}, \ j = 1, 2, \ldots, k \), are the corresponding eigenvectors. Because the Gauss–Christoffel quadrature is exact for polynomials up to degree \( 2k - 1 \), we have

\[
\int_{-\infty}^{\infty} \lambda^i d\lambda^{(k)}(\lambda) = \sum_{i=1}^{k} w_{j}^{(k)} \{ \lambda_j^{(k)} \}^i = \mathbf{e}_1^T (T_{k,k})^i \mathbf{e}_1, \quad \lambda = 0, 1, \ldots, 2k - 1,
\]

and the first \( 2k \) moments match

\[
\mathbf{v}^H A^i \mathbf{v} = \mathbf{e}_1^T (T_{k,k})^i \mathbf{e}_1, \quad \lambda = 0, 1, \ldots, 2k - 1.
\]  

(2.6)

2.2 Model reduction via Vorobyev moment matching

We can state the problem of moment matching in the language of matrices via the Vorobyev moment problem. We follow [Vorobyev (1963)] for the derivation of a linear operator \( S_k \) given by reducing the model order of \( S = \mathbf{z}^T - \mathbf{A} \). (See also [Brezinski (1996)] and [Strakoš (2009)].) First, we derive a linear operator \( A_k \) that reduces the model order of \( A \). Let

\[
\begin{align*}
\mathbf{z}_1 &= \mathbf{A} \mathbf{v}, \\
\mathbf{z}_2 &= \mathbf{A} \mathbf{z}_1 (= \mathbf{A}^2 \mathbf{v}), \\
&\vdots \\
\mathbf{z}_{k-1} &= \mathbf{A} \mathbf{z}_{k-2} (= \mathbf{A}^{k-1} \mathbf{v}), \\
\mathbf{z}_k &= \mathbf{A} \mathbf{z}_{k-1} (= \mathbf{A}^k \mathbf{v}),
\end{align*}
\]

where \( \mathbf{v}, \mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_k \) are assumed to be linearly independent. Then, the Vorobyev moment problem involves determining a sequence of linear operators \( A_k \) such that

\[
\begin{align*}
\mathbf{z}_1 &= \mathbf{A}_k \mathbf{v}, \\
\mathbf{z}_2 &= \mathbf{A}_k \mathbf{z}_1 (= \mathbf{A}_k^2 \mathbf{v}), \\
&\vdots \\
\mathbf{z}_{k-1} &= \mathbf{A}_k \mathbf{z}_{k-2} (= \mathbf{A}_k^{k-1} \mathbf{v}), \\
Q_k \mathbf{z}_k &= \mathbf{A}_k \mathbf{z}_{k-1} (= \mathbf{A}_k^k \mathbf{v}),
\end{align*}
\]
where \( Q_k = V_k V_k^H \) is the orthogonal projector onto \( K_k(A,v) \). A linear operator \( A_k \) reducing the model order of \( A \) is given by

\[
A_k = Q_k A Q_k = V_k T_{k,k} V_k^H, \tag{2.7}
\]

where the sequence \( \{ A_k \}_{k \geq 0} \) is strongly convergent to \( A \) \footnote{Vorobyev, 1965, Theorem II). (See Brezinski, 1996, Section 4.2) for the derivation of (2.7).} Hence, the first \( 2k \) moments of the reduced model match those of the original model

\[
v^H A^i v = v^H (A_k)^i v = (v^H v) e_1^H (T_{k,k})^i e_1, \quad i = 0, 1, \ldots, 2k - 1. \tag{2.8}
\]

See Appendix A for the derivation of (2.8).

### 3 Shifted Lanczos method

Next, we formulate a shifted Lanczos method. Application of Vorobyev’s method of moments to the shifted matrix \( zI - A \) and vector \( v \) gives a matrix representation of a linear operator that represents the reduced model to approximate the resolvent \((zI - A)^{-1}\). We first solve the problem for the linear operator \( S_k \). Let

\[
\begin{align*}
z_1 &= Sv, \\
z_2 &= Sz_1 = (S^2)v, \\
&\vdots \\
z_{k-1} &= Sz_{k-2} = (S^{k-1})v, \\
z_k &= Sz_{k-1} = (S^k)v,
\end{align*}
\]

where \( v, z_1, z_2, \ldots, z_k \) are assumed to be linearly independent. Then, the Vorobyev moment problem involves determining a sequence of linear operators \( S_k \) such that

\[
\begin{align*}
z_1 &= S_k v, \\
z_2 &= S_k z_1 = (S_k^2)v, \\
&\vdots \\
z_{k-1} &= S_k z_{k-2} = (S_k^{k-1})v, \\
Q_k z_k &= S_k z_{k-1} = (S_k^k)v,
\end{align*}
\]

where \( Q_k = V_k V_k^H \) is the orthogonal projector onto \( K_k(S,v) \). Equations (3.1) can be written as

\[
z_i = (S_k)^i v, \quad i = 1, 2, \ldots, k - 1, \quad Q_k z_k = (S_k^k)v.
\]

An arbitrary vector in \( K_k(S,v) \) has the expansion

\[
u = \sum_{i=0}^{k-1} a_i z_i, \quad a_i \in \mathbb{C},
\]

where \( z_0 = v \). Multiplying both sides by \( S \), we have

\[
Su = \sum_{i=0}^{k-2} a_i S^{i+1} v + a_{k-1} S z_k.
\]
Projecting this onto $K_k(S,v) = K_k(A,v)$, we have

$$Q_k S u = \sum_{i=0}^{k-2} a_i (S_k)^{i+1} v + a_{k-1} (S_k)^{k} v$$

$$= \sum_{i=0}^{k-1} a_i (S_k)^{i+1} v$$

$$= \sum_{i=0}^{k-1} a_i S_k z_i$$

$$= S_k u.$$  

Here, the first equality is due to

$$Q_k S^i v = Q_k S^{i+1} v$$

$$= S^{i+1} v \in K_k(S,v), \quad i = 0, 1, \ldots, k - 2.$$  

This shows that $Q_k S = S_k$ on $K_k(S,v)$. Since $Q_k w \in K_k(S,v)$ for $w \in \mathbb{C}^n$, we can obtain the expression

$$S_k = Q_k S Q_k$$

by extending the domain to the whole space $\mathbb{C}^n$.

Using the expression $S_k$, we show that the moments of the original model with $zI - A$ and $v$ and those of the reduced model with $zI - T_{k,k}$ and $e_1$ match. Subtracting (2.1) from the identity $zV_k = zV_{k+1} \left[ \begin{array}{c} 1 \\ 0^T \end{array} \right]$, we obtain the Lanczos-like decomposition

$$(zI - A)V_k = V_{k+1} \left( z \left[ \begin{array}{c} 1 \\ 0^T \end{array} \right] - T_{k+1,k} \right).$$  \hspace{1cm} (3.2)$$

Note that direct application of the Lanczos method to $zI - A$ does not necessarily give the decomposition (3.2). Multiplying this by $V_k^H$, we have

$$V_k^H (zI - A) V_k = zI - T_{k,k}.$$  

This gives the orthogonally projected restriction

$$S_k = V_k V_k^H (zI - A) V_k V_k^H$$

$$= V_k (zI - T_{k,k}) V_k^H.$$  

Note that the sequence $\{S_k\}_{k \geq 0}$ is strongly convergent to $S$ (Vorobyev, 1965, Theorem II). By using the matching moments for $A$ and the binomial formula, we have

$$v^H (zI - A)^i v = \sum_{j=0}^{i} \binom{i}{j} z^{i-j} (-1)^j v^H A^j v$$

$$= \sum_{j=0}^{i} \binom{i}{j} z^{i-j} (-1)^j v^H (A_k)^j v$$

$$= v^H (zI - A_k)^i v, \quad i = 0, 1, \ldots, 2k - 1,$$

where $\binom{i}{j}$ denotes the binomial coefficient. Therefore, the reduced model matches the first $2k$ moments of the original model

$$v^H S^i v = v^H (S_k)^i v$$

$$= (v^H v) e_1^\top (zI - T_{k,k})^i e_1, \quad i = 0, 1, \ldots, 2k - 1.$$
Note that the left-hand side is equal to
\[ \sum_{j=0}^{i} w_j (z - \lambda_j)^i = \int_{-\infty}^{\infty} (z - \lambda)^i d\omega(\lambda) \]
with distribution function \( (2.4) \) and the right-hand side is equal to
\[ \sum_{j=0}^{i} w_j (z - \lambda_j^{(k)})^i = \int_{-\infty}^{\infty} (z - \lambda)^i d\omega^{(k)}(\lambda) \]
with distribution function \( (2.5) \) (cf. Szegö, 1959, Chapter 15).

Let us now come back to the approximation of \( v^H S^{-1} v \). Because
\[ S_k^{-1} = V_k (z I - T_{k,k})^{-1} V_k^H \]
is the matrix representation of the inverse of the reduced-order operator \( S_k \) restricted onto \( K_k(S, v) \) (Hoffman & Kunze, 1971, p. 79), an approximation is given by \( v^H (S_k)^{-1} v \). Hence, we have
\[ v^H (S_k)^{-1} v = (v^H v) e_1^\top (z I - T_{k,k})^{-1} e_1 \equiv L_k(z). \]  
\[ (3.3) \]

### 3.1 Implementation

The quantity \( (3.3) \) is the \((1,1)\) entry of the resolvent of a successively enlarging tridiagonal matrix. An efficient recursive formula for computing such an entry was developed in [Golub & Meurant] (2010, Section 3.4). The \((1,1)\) entry \( L_k(z) \) of the resolvent \((z I - T_{k,k})^{-1}\) for the successively enlarging Jacobi matrix \( T_{k,k} \) is recursively computed with \( c_1 = 1, \delta_1 = z - \alpha_1, \pi_1 = 1/\delta_1 \) using
\[ L_{k+1}(z) = L_k(z) + c_{k+1} \pi_{k+1}, \quad k = 1, 2, \ldots, \]
where \( T_{k,k} = (\beta_k)^2 \pi_k, \delta_{k+1} = z - \alpha_{k+1} - T_{k,k}, \pi_{k+1} = 1/\delta_{k+1} \) and \( c_{k+1} = c_k T_{k,k} \pi_k \), as given in Algorithm 3.1. We summarise the procedures for approximating quadratic forms \((1.1)\). The difference from Algorithm \((2.1)\) is the addition of Lines 2 and 7. In particular, when \( A \) is a real symmetric matrix and \( v \) is a real vector in Algorithm \((3.1)\) only real arithmetic is needed to compute Lines 1, 4 and 6, whereas Lines 2 and 7 require complex arithmetic.

**Algorithm 3.1** Shifted Lanczos method for quadratic forms

**Input:** \( A \in \mathbb{C}^{n \times n}, v \in \mathbb{C}^n, z_i \in \mathbb{C}, i = 1, 2, \ldots, m \)

**Output:** \( L_k(z_i) \in \mathbb{C}, i = 1, 2, \ldots, m \)

1. \( v_1 = v/\|v\|, \quad u = Av_1, \quad \alpha_1 = u^H v_1 \)
2. \( c_1^{(i)} = v_1^\top u, \quad \delta_1^{(i)} = z_i - \alpha_1, \quad \pi_1^{(i)} = 1/\delta_1^{(i)}, \quad L_1(z_i) = c_1^{(i)}/(z_i - \alpha_1), i = 1, 2, \ldots, m \)
3. for \( k = 1, 2, \ldots, \) until convergence do 
   4. \( u = u - \alpha_k v_k, \quad \beta_k = \|u\| \)
   5. if \( \beta_k = 0 \) then break
   6. \( v_{k+1} = (\beta_k)^{-1} u, \quad u = Av_{k+1} - \beta_k v_k, \quad \alpha_{k+1} = u^H v_{k+1} \)
   7. \( t_k^{(i)} = (\beta_k)^2 \pi_k^{(i)}, \quad \delta_k^{(i)} = z_i - \alpha_{k+1} - t_k^{(i)}, \quad \pi_k^{(i)} = 1/\delta_k^{(i)}, \quad c_{k+1}^{(i)} = c_k^{(i)} t_k^{(i)} / \pi_k^{(i)}, \quad L_{k+1}(z_i) = L_k(z_i) + c_{k+1}^{(i)} \pi_{k+1}^{(i)}, i = 1, 2, \ldots, m \)
8. end for

We compare the shifted Lanczos method with related methods in terms of computational cost. Algorithms \((3.2), (3.3)\) and \((3.4)\) give simple modifications of the shifted COCG, COCR and MINRES methods, respectively, for computing quadratic forms \((1.1)\). Here, \( z_s \) is the seed shift that can be chosen among the target shifts \( z_i, i = 1, 2, \ldots, m \). The modifications are given by
applying \( \mathbf{v}^\top \) to the \( k \)th iterate \( \mathbf{x}_k \) and associated vectors. They produce approximations \( G_k(z_i) \), \( R_k(z_i) \) and \( M_k(z_i) \), respectively, to the quadratic form (1.1). Note that the shifted COCG and COCR methods use complex arithmetic throughout for \( \mathbf{v} \in \mathbb{C}^n \setminus \mathbb{R}^n \) or \( z_i \in \mathbb{C} \setminus \mathbb{R} \), whereas the shifted MINRES method uses real arithmetic to compute the matrix–vector product \( A\mathbf{q}_k \) for real \( A \) and \( \mathbf{v} \), similarly to the shifted Lanczos method.

For simplicity of comparison, we count basic vector and matrix operations. The Lanczos method (Algorithm 2.1) needs one vector scale (scale), one dot product (dot), one vector norm (norm), two scalar–vector additions (axpy) and one matrix–vector product (matvec) per iteration. Table 3.1 gives the number of basic vector and matrix operations of the shifted methods. Table 3.2 gives the number of scalar operations for each shift \( z_i \) per iteration. These tables show that in terms of the cost per iteration, the shifted Lanczos method is the cheapest of the methods compared.

**Algorithm 3.2** Shifted COCG method for quadratic forms

\[
\begin{align*}
\text{Input:} & \quad A \in \mathbb{R}^{n \times n}, \mathbf{v} \in \mathbb{C}^n, z_s \in \mathbb{C}, z_i \in \mathbb{C}, i = 1, 2, \ldots, m \\
\text{Output:} & \quad G_k(z_i) \in \mathbb{C}, i = 1, 2, \ldots, m
\end{align*}
\]

1. \( \alpha_{i-1} = 1, \beta_{i-1} = 0, p_{i-1} = 0, r_0 = \mathbf{v} \)
2. \( \pi_{i}^{(i)} = \pi_{0}^{(i)} = 1, p_{0}^{(i)} = \mathbf{v}^\top r_0, G_0(z_i) = 0, i = 1, 2, \ldots, m \)
3. for \( k = 1, 2, \ldots, \) until convergence do
   4. \( p_{k-1} = r_{k-1} + \beta_{k-2}p_{k-2} \)
   5. if \( p_{k-1}^\top (z_s I - A) p_{k-1} = 0 \) or \( r_{k-1}^\top r_{k-1} = 0 \) then switch the seed
   6. \( \alpha_{k-1} = (r_{k-1}^\top r_{k-1})/(p_{k-1}^\top (z_s I - A) p_{k-1}), r_k = r_{k-1} - \alpha_{k-1}(z_s I - A) p_{k-1}, \beta_{k-1} = (r_k^\top r_k)/(r_{k-1}^\top r_{k-1}), r_k = \mathbf{v}^\top r_k \)
   7. for \( i = 1, 2, \ldots, m \) do
      8. \( \pi_{i}^{(i)} = [1 + \alpha_{k-1}(z_i - z_s) + (\beta_{k-2}/\alpha_{k-2}) \alpha_{k-1}] \pi_{k-1}^{(i)} - (\beta_{k-2}/\alpha_{k-2}) \alpha_{k-1} \pi_{k-2}^{(i)} \)
      9. if \( \pi_{i}^{(i)} = 0 \) then output \( G_{k-1}(z_i) \)
   10. \( \alpha_{k-1}^{(i)} = (\pi_{k-1}^{(i)}/\pi_k^{(i)}) \alpha_{k-1}, \beta_{k-1}^{(i)} = (\pi_{k-1}^{(i)}/\pi_k^{(i)})^2 \beta_{k-1}, r_k^{(i)} = r_k/\pi_k^{(i)}, G_k^{(i)}(z_i) = G_{k-1}(z_i) + \alpha_{k-1}^{(i)} p_{k-1}^{(i)}, p_k^{(i)} = r_k^{(i)} + \beta_{k-1}^{(i)} p_{k-1}^{(i)} \)
   11. end for
12. end for

3.2 Breakdown-free condition

A breakdown resulting from division by zero for \( \delta_{k+1}^{(i)} = 0 \) may occur in Line 7 of Algorithm 3.1. Therefore, we give a sufficient condition such that the shifted Lanczos method does not break down. Let \( T_k^\leq = z I - T_{k,k} \) with \( z \in \mathbb{C} \) and \( |T_0^\leq| = 1 \) for convenience, where \( | \cdot | \) denotes the determinant of a matrix. For convenience, we omit superscript \( (i) \) from quantities given in Algorithm 3.1 and prepare lemmas.

**Lemma 3.1.** Let \( \alpha_k, \beta_k \) and \( T_k^\leq \) be defined as above. Then we have

\[
|T_{k+1}^\leq| = (z - \alpha_{k+1})|T_k^\leq| - (\beta_k)^2|T_{k-1}^\leq|, \quad k \in \mathbb{Z}_{>0}.
\]

**Proof.** The Laplace expansion of \( |T_{k+1}^\leq| \) by minors along the last column and the alternating
Algorithm 3.3 Shifted COCR method for quadratic forms

Input: $A \in \mathbb{R}^{n \times n}$, $v \in \mathbb{C}^n$, $z_s \in \mathbb{C}$, $z_i \in \mathbb{C}$, $i = 1, 2, \ldots, m$

Output: $R_k(z_i) \in \mathbb{C}$, $i = 1, 2, \ldots, m$

1: $\alpha_{-1} = 1$, $\beta_{-1} = 0$, $q_{-1} = 0$, $r_0 = v$, $r_0 = v^H r_0$
2: $p_{-1} = 0$, $\pi_{-1} = \pi_0 = 1$, $r_0 = v$, $p_0 = v^H r_0$, $R_0(z_i) = 0$, $i = 1, 2, \ldots, m$
3: for $k = 1, 2, \ldots$, until convergence do
4: $q_{k-1} = (z_s I - A)r_{k-1} + \beta_{k-2} q_{k-2}$
5: if $q_{k-1} = 0$ then switch the seed
6: $\alpha_{k-1} = [r_{k-1}^T (z_s I - A)]/[q_{k-1}^T q_{k-1}]$
7: for $i = 1, 2, \ldots, m$ do
8: $\pi_k = (1 + (\beta_{k-2}/\alpha_{k-2}) \alpha_{k-1} + \alpha_{k-1}(z_s - z_s)) \pi_{k-1} - (\beta_{k-2}/\alpha_{k-2}) \alpha_{k-1} \pi_{k-2}$
9: if $\pi_k = 0$ then output $R_k(z_i)$
10: $\beta_{k-2} = (\pi_{k-2}/\pi_{k-1})^2$, $\alpha_{k-1} = (\pi_k/\pi_{k-1}) \alpha_{k-1}$, $p_{k-1} = r_{k-1} - \beta_{k-2} p_{k-2}$
11: $R_k^i = R_{k-1} + \alpha_{k-1} p_{k-1}$
12: end for
13: $r_k = r_{k-1} - \alpha_{k-1} q_{k-1}$, $r_k = v^H r_k$
14: if $r_{k-1}^T (z_s I - A)r_{k-1} = 0$ then switch the seed
15: $\beta_{k-1} = [r_k^T (z_s I - A) r_k] / [r_{k-1}^T (z_s I - A) r_{k-1}]$
16: end for

Algorithm 3.4 Shifted MINRES method for quadratic forms

Input: $A \in \mathbb{C}^{n \times n}$, $v \in \mathbb{C}^n$, $x_0 \in \mathbb{C}^n$, $z_s \in \mathbb{C}$, $z_i \in \mathbb{C}$, $i = 1, 2, \ldots, m$

Output: $M_k(z_i) \in \mathbb{C}$, $i = 1, 2, \ldots, m$

1: $\beta_0 = 0$, $q_0 = 0$, $r_0 = v - (z_s I - A)x_0$, $q_1 = \|r_0\|^{-1} r_0$, $q_1 = v^H q_1$
2: $p_1^T = 1$, $t_k = s_k - \alpha_k q_k$, $f_k = \|t_k\|$, $g_k = v^H q_k$
3: for $k = 1, 2, \ldots$, until convergence do
4: $s_k = A^k - \beta_k - 1 q_{k-1}$, $\alpha_k = s_k^H q_k$, $t_k = s_k - \alpha_k q_k$, $\beta_k = \|t_k\|$, $q_k = v^H q_k$
5: for $i = 1, 2, \ldots, m$ do
6: $r_{k-2i} = 0$, $r_{k-1} = \beta_{k-1}$, $r_{i,k} = z_i - \alpha_k$
7: if $k \geq 3$ then update $[r_{k-2i,k}^T, r_{k-1,k}^T] = C_{k-2}^i [r_{k-2i,k}, r_{k-1,k}]^T$
8: if $k \geq 2$ then update $[r_{k-1,k}^T, r_{k,k}^T] = C_k^i [r_{k-1,k}, r_{k,k}]^T$
9: Compute $G_i^k = \begin{bmatrix} c_i^k & s_i^k \\ -s_i^k & c_i^k \end{bmatrix}$ and update $r_{k,k}$ such that $[r_{k,k}^T, 0]^T = G_i^k [r_{k,k}, \beta_k]^T$, $|c_i^k|^2 + |s_i^k|^2 = 1$, $c_i^k, s_i^k \in \mathbb{C}$.
10: if $s_i^k = 0$ then output $M_i^k$
11: $p_i = (r_{k,k}^T)^{-1} (q_k - r_{k-2i,k} p_{k-2} - r_{k-1,k} p_{k-1})$, $M_k(z_i) = M_{k-1}(z_i) + \|r_0\| c_i^k f_k^T p_k$, $f_{k+1}^T = -s_i^k f_k^T$
12: end for
13: $q_{k+1} = (\beta_k)^{-1} t_k$
14: end for
Table 3.1: Basic vector and matrix operations

| Method          | scale | dot | norm | axpy | matvec |
|-----------------|-------|-----|------|------|--------|
| Shifted Lanczos | 1     | 1   | 1    | 2    | 1      |
| Shifted COCG    | 1     | 1   | 1    | 2    | 1      |
| Shifted COCR    | 0     | 3   | 0    | 2    | 1      |
| Shifted MINRES  | 1     | 2   | 1    | 2    | 1      |

Method: name of the method, scale: vector scale, dot: dot product, norm: vector norm, axpy: scalar–vector addition, matvec: matrix–vector product.

Table 3.2: Scalar operations for each shift $z_i$ per iteration

| Method          | +  | ×  | /  | √  | Total |
|-----------------|----|----|----|----|-------|
| Shifted Lanczos | 3  | 4  | 1  | 0  | 8     |
| Shifted COCG    | 6  | 9  | 3  | 0  | 18    |
| Shifted COCR    | 6  | 8  | 3  | 0  | 17    |
| Shifted MINRES  | 11 | 20 | 3  | 1  | 35    |

Method: name of the method, +: addition, ×: multiplication, /: division, √: square root, Total: total number of operations.

property of matrix determinants give

$$|T_{k+1}^<| = \begin{vmatrix} T_k^< & 0 \\ 0 & -\beta_k \end{vmatrix} = \begin{vmatrix} T_{k-1}^< & 0 \\ 0 & -\beta_{k-1} \end{vmatrix} = (z - \alpha_{k+1})|T_k^<| + \beta_k |T_{k-1}^<| = (z - \alpha_{k+1})|T_k^<| - (\beta_k)^2|T_{k-1}^<|.$$  

Lemma 3.2. Let $\delta_k$ and $T_k^<$ be defined as above. If $|T_i^<| \neq 0$, $i = 1, 2, \ldots, k$, then we have

$$\delta_{k+1} = \frac{|T_{k+1}^<|}{|T_k^<|}, \quad k \in \mathbb{Z}_{>0}.$$  

Proof. We prove the assertion by induction. Assume $|T_1^<| \neq 0$. Then it follows from the definition that

$$\delta_2 = z - \alpha_2 - (\beta_1)^2 \frac{1}{\delta_1} = \frac{(z - \alpha_1)(z - \alpha_2) - (\beta_1)^2}{z - \alpha_1}.$$
holds. On the other hand, \(|T_1^<| = z - \alpha_1\) and \(|T_2^<| = (z - \alpha_1)(z - \alpha_2) - (\beta_1)^2\) hold. Hence, the assertion holds for \(k = 1\). Assume that \(|T_i^<| \neq 0\) holds for \(i = 1, 2, \ldots, k\) and \(\delta_k = |T_k^<|/|T_{k-1}^<|\) holds for \(k > 1\). Then Lemma 3.1 gives

\[
\delta_{k+1} = z - \alpha_{k+1} - t_k = z - \alpha_{k+1} - (\beta_k)^2 \frac{|T_{k-1}^<|}{|T_k^<|} = z - \alpha_{k+1} - \frac{z - \alpha_{k+1} |T_k^<| - |T_{k+1}^<|}{|T_k^<|} = \frac{|T_{k+1}^<|}{|T_k^<|}.
\]

\[\square\]

**Lemma 3.3.** Let \(T_k^<\) and \(\delta_k\) be defined as above. Assume that \(|T_i^<| \neq 0\) holds for \(i = 1, 2, \ldots, k\), \(k \in \mathbb{Z}_{>0}\). If \(\delta_{k+1} = 0\) for \(k \in \mathbb{Z}_{>0}\), then we have \(|T_{k+1}^<| = 0\).

**Proof.** The condition \(\delta_{k+1} = 0\) gives \(t_k = z - \alpha_{k+1}\). It follows from Lemmas 3.1 and 3.2 that

\[
|T_{k+1}^<| = |T_k^<| \left(z - \alpha_{k+1} - (\beta_k)^2 \frac{|T_{k-1}^<|}{|T_k^<|}\right) = |T_k^<| (z - \alpha_{k+1} - t_k) = 0.
\]

\[\square\]

s orthogonal to the vector

We are ready to give the breakdown-free condition.

**Theorem 3.4.** Let \(\delta_k\) be defined as above. Let \(\lambda_1\) and \(\lambda_n\) be the smallest and largest eigenvalues of \(A\), respectively. If \(z \in \mathbb{C}\) satisfies \(z \notin [\lambda_1, \lambda_n]\), then \(\delta_k \neq 0\) holds for \(k \in \mathbb{Z}_{>0}\).

**Proof.** From the interlacing property (Horn & Johnson 2013, Theorem 4.3.17), \(T_{k,k}\) does not have an eigenvalue equal to \(z\). Hence, \(|T_k^<| \neq 0\) holds. From Lemma 3.3, the assertion holds. \[\square\]

Theorem 3.4 shows that the shifted Lanczos method does not break down, whenever each \(z_i \in \mathbb{C}\) satisfies \(z_i \notin [\lambda_1, \lambda_n]\).

### 4 Numerical experiments

Numerical experiments compare the proposed method with previous methods in terms of the number of iterations and CPU time. The methods compared are the shifted COCR method (Algorithm 3.3), shifted MINRES method (Algorithm 3.4) and shifted Lanczos method (Algorithm 3.1, as well as the direct solver using the MATLAB function \texttt{mldivide} for solving (1.2).

All computations were performed on a computer with an Intel Xeon E5-2670 v2 2.50 GHz CPU, 256 GB of random-access memory (RAM) and CentOS 6.10. All programs were coded and run in MATLAB R2019a in double-precision floating-point arithmetic with unit round-off at \(2^{-52} \approx 2.2 \cdot 10^{-16}\).

Table 4.1 gives information about the test matrices, including the size of each matrix, density of the non-zero entries [\%], (estimated) condition number and application from which the matrix arose. The condition number was estimated using the MATLAB function \texttt{condest}. Matrices apache2, CurlCurl_3 and thermal2 are from Davis & Hu (2011); the other matrix,
Table 4.1: Information on test matrices

| Matrix         | n            | Density [%] | condest       | Application               |
|---------------|--------------|-------------|---------------|---------------------------|
| apache2       | 715,176      | 9.4 · 10^{-4} | 5.3 · 10^6   | Structural analysis       |
| VCNT1000000std| 1,000,000    | 4.0 · 10^{-3} | 1.2 · 10^2   | Quantum chemistry         |
| CurlCurl_3    | 1,219,574    | 9.1 · 10^{-4} | —            | Electromagnetic analysis  |
| thermal2      | 1,228,045    | 5.7 · 10^{-4} | 7.5 · 10^6   | Steady-state thermal analysis |

Matrix: name of the matrix, n: size of the matrix, density: density of nonzero entries, condest: condition number estimated by using the MATLAB function condest, application: application from which the matrix arises.

VCNT1000000std, is from [Hoshi et al. (2019)]. They are sparse symmetric matrices. The condition number for CurlCurl_3 could not be computed because of insufficient computer memory. Vector $\mathbf{v}$ was set to $\mathbf{v} = (1/n)\mathbf{e}$ for reproducibility, where $\mathbf{e}$ is the all-ones vector. The shifts were set to $z_i = \exp\left(-\frac{2i + 1}{2m}\pi\right)$, $i = 1, 2, \ldots, m$, $m = 16$.

4.1 Comparisons in terms of CPU time

We compare the methods in terms of CPU time. Figure 4.1 shows the relative error versus the number of iterations for test matrices. The shifted Lanczos method converged faster than the other methods on apache2 and thermal2 and was competitive with the shifted MINRES method on VCNT1000000std. The shifted Lanczos method was faster than the other methods on CurlCurl_3 near the stopping criterion and stagnated without convergence. The shifted COCR and MINRES methods were almost identical on CurlCurl_3. The convergence curves of the four methods on VCNT1000000std and CurlCurl_3 decreased monotonically. Although the shifted MINRES method is monotonically non-increasing in terms of the residual norm, plots 4.1a and 4.1d show that the shifted MINRES method does not necessarily converge monotonically in terms of the error. The convergence curves of the four methods are oscillatory on apache2 and thermal2. The shifted Lanczos method did not reach the stopping criterion on CurlCurl_3 whereas the shifted COCR and MINRES methods did.

Table 4.2 gives the CPU time in seconds taken by the four methods. MATLAB’s sparse direct solver gave values for the largest relative residual norm $\max_i \|\mathbf{v} - (z_i I - A)\hat{\mathbf{x}}^{(i)}\|/\|\mathbf{b}\|$ of $4.6 \cdot 10^{-12}$, $9.4 \cdot 10^{-16}$, $5.0 \cdot 10^{-12}$ and $6.4 \cdot 10^{-16}$ among $i = 1, 2, \ldots, m$ for apache2, VCNT1000000std, CurlCurl_3 and thermal2, respectively, where $\hat{\mathbf{x}}^{(i)}$ is the numerical solution of linear system $(z_i I - A)x^{(i)} = \mathbf{b}$. The sparse direct solver was accurate on VCNT1000000std and thermal2 and not accurate on apache2 and CurlCurl_3.

The shifted methods terminated when the largest relative error became less than or equal to $10^{-10}$. The shifted Lanczos method was competitive with or faster than the MINRES method except on CurlCurl_3 whereas the shifted COCR method took more CPU time; this is because the complex arithmetic for computing the matrix–vector product in the shifted COCR method is time consuming.

4.2 Estimation of error

To terminate the iteration of Algorithm 3.1 once a satisfactory solution is obtained, we propose using an estimate

$$\hat{\nu}_{k,d} = (\mathbf{v}^H\mathbf{v})[\mathbf{e}_1^\top(T_{k+d}^\infty)^{-1}\mathbf{e}_1 - \mathbf{e}_1^\top(T_{k}^\infty)^{-1}\mathbf{e}_1],$$

of the error for the $k$th iteration in practice. This estimate is an analogous formula of $\nu_{k,d} = (\mathbf{v}^H\mathbf{v})[\mathbf{e}_1^\top(T_{k+d,k+d}^\infty)^{-1}\mathbf{e}_1 - \mathbf{e}_1^\top(T_{k,k}^\infty)^{-1}\mathbf{e}_1]$ (Strakoš & Tichý 2002, Section 4) for the error in
the conjugate gradient (CG) method, in which it is supposed that the approximation error for the $(k + d)$th iteration is significantly smaller than that for the $k$th iteration.

We present the estimate on the matrices used in Section 4.1. Figure 4.2 shows the relative error versus the number of iterations and its estimate $\hat{\nu}_{k,d}$ with $d = 5$. Here, we chose two shifts $z_i$ for $i = 1, 9$ in (4.1); one is closest to the real axis and the other is farthest from the real axis among the shifts $z_i$ for $i = 1, 2, \ldots, 16$. The error was accurately estimated for VCNT1000000std and thermal2. The error was underestimated for apache2 and CurlCurl_3 because although the quantity $\nu_{k,d}$ estimates the error to a certain extent, the shifted Lanczos method lacks the monotonicity of an error norm such as the one in the CG method (cf. Strakos & Tichý, 2002). The oscillations of the estimates are similar to those observed in the errors for apache2 and thermal2.

Figure 4.1: Relative error vs number of iterations.

Table 4.2: CPU times [seconds] on test matrices for the methods compared

| Method    | apache2 | VCNT1000000std | CurlCurl_3 | thermal2 |
|-----------|---------|----------------|-------------|----------|
| mldivide  | 1,978   | 555            | 749,696     | 563      |
| Shifted COCR | 292     | 3.60           | 574         | 30.3     |
| Shifted MINRES | 130     | 1.45           | 234         | 10.2     |
| Shifted Lanczos | 96.1    | 1.49           | —           | 10.2     |
Figure 4.2: Relative error and its estimate \( \hat{\nu}_{k,d} \) with \( d = 5 \) vs number of iterations.

5 Conclusions

We explored the computation of quadratic forms of Hermitian matrix resolvents. In contrast to previous Krylov subspace methods that use the shift-invariance property for solving shifted linear systems, our method approximates the matrix resolvent directly. The underlying concept used in approximating the resolvent is to exploit the moment-matching property of a shifted Lanczos method via solving the Vorobyev moment problem. We showed that the shifted Lanczos method matches the first \( k \) moments of the original model and those of the reduced model and extended the scope of the problems that the standard Lanczos method can solve. We derived the inverse of a linear operator representing the reduced model and related it to an entry of a Jacobi matrix resolvent. The entry can be efficiently computed by using a recursive formula. Previous shifted Krylov subspace methods work on a real symmetric matrix with a complex shift, whereas the proposed method works on a Hermitian matrix with a complex shift and does not break down, provided that the shift is not in the interior of the extremal eigenvalues of the Hermitian matrix. Numerical experiments on matrices drawn from real-world applications showed that the shifted Lanczos method is competitive with the shifted MINRES method and outperforms it when solving some problems. We demonstrated that an analogue of a previous error estimation formula for the conjugate gradient method is reasonable.

We intend to extend the solution for the single-vector case \( v \) to the multiple-vector case (cf. [Golub & Meurant, 2010, p. 114]) and perform preconditioning for the shifted Lanczos method for future work. The COCG and COCR methods can use preconditioning if the preconditioned matrix is complex symmetric; however, for the shifted Lanczos method, it is not trivial to incorporate preconditioning. It is also not trivial how to monitor the convergence of the proposed method, and we leave the development of a more rigorous and/or sophisticated estimate for future. With regard to the error estimate, there will be an interesting connection with the
Gauss quadratures (cf. Golub & Meurant [1993, 1997] Meurant & Tichý [2013]).

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