WHEN DOES THE LANCZOS ALGORITHM COMPUTE EXACTLY?

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Abstract. In theory, the Lanczos algorithm generates an orthogonal basis of the corresponding Krylov subspace. However, in finite precision arithmetic, the orthogonality and linear independence of the computed Lanczos vectors is usually lost quickly. In this paper we study a class of matrices and starting vectors having a special nonzero structure that guarantees exact computations of the Lanczos algorithm whenever floating point arithmetic satisfying the IEEE 754 standard is used. Analogous results are formulated also for a variant of the conjugate gradient method that produces then almost exact results. The results are extended to the Arnoldi algorithm, the nonsymmetric Lanczos algorithm, the Golub-Kahan bidiagonalization, the block-Lanczos algorithm and their counterparts for solving linear systems.

Key words. Lanczos algorithm, exact computations, finite precision arithmetic, rounding errors

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1. Introduction. Let a real and symmetric matrix $A$ and a starting vector $v$ be given. The Lanczos algorithm is a frequently used algorithm for computing an orthogonal basis of the corresponding Krylov subspace. At the same time, it can be seen as a method for approximating a few eigenvalues (and eventually eigenvectors) of $A$, using the underlying Rayleigh-Ritz procedure; see, e.g., [25].

Since the introduction of the algorithm in 1950 by Lanczos [17] it has been known that the orthogonality of the computed basis vectors need not be preserved due to rounding errors. As a consequence, an eigenvalue of $A$ can be approximated by several eigenvalues of the Jacobi matrix produced by the Lanczos algorithm in finite precision arithmetic.

The numerical behavior of the Lanczos algorithm was analyzed by Paige [22, 23]. Paige showed that the effects of rounding errors on the Lanczos algorithm can be described mathematically. Based on these results, Greenbaum [10] proved that the results of finite precision computations can be interpreted as the results of the exact Lanczos algorithm applied to a larger problem with a matrix having many eigenvalues distributed throughout tiny intervals around the eigenvalues of $A$. In other words, Greenbaum found and constructed a mathematical model of the finite precision Lanczos computations. In particular, Greenbaum’s model matrix is a Jacobi matrix, and the starting vector is a multiple of the first column $e_1$ of the identity matrix. Results of Paige and Greenbaum stimulated further development in the analysis of the numerical behavior of the Lanczos and the conjugate gradient (CG) algorithms; see, e.g., [28, 12, 30, 29]. For a comprehensive summary and a detailed explanation; see [20].

In this paper we extend an interesting observation made by Marie Kubínová in her PhD thesis [16, p. 77]: If the Lanczos algorithm is applied to a Jacobi matrix and a multiple of $e_1$, then no rounding errors appear. In other words, the finite precision Lanczos algorithm computes exactly. Note that we also formulate analogous statement for a variant of the CG algorithm that provides, for the above mentioned input data, almost exact results (within the relative accuracy given by machine precision). The obtained results have several consequences discussed in detail in Section 7, that could be useful in further analysis of the behavior of the Lanczos and CG algorithms. For example, they allow to investigate experimentally the theoretical behavior of the Lanczos algorithm for potentially very large systems by forming a tridiagonal matrix with the desired properties, and then running the Lanczos algorithm with the starting vector $e_1$ without reorthogonalization.

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The paper is organized as follows. In Sections 2 and 3 we recall the standard version of the Lanczos algorithm, and summarize operations and transformations that are performed exactly in floating point arithmetic. Section 4 investigates a nonzero structure of the input data, that ensures the exact computations of the Lanczos algorithm in floating point arithmetic satisfying the IEEE 754 standard. In Section 5 we formulate analogous results for a variant of the CG method. Section 6 shows that the results of Sections 4 and 5 can be generalized to other algorithms like the Arnoldi algorithm, the nonsymmetric Lanczos algorithm, the Golub-Kahan bidiagonalization and the block-Lanczos algorithm and their counterparts for solving linear systems. Finally, in Section 7 we discuss consequences and a possible use of the obtained results.

2. Lanczos algorithm. Given a starting vector \( v \in \mathbb{R}^n \) and a symmetric matrix \( A \in \mathbb{R}^{n \times n} \), one can consider a sequence of nested subspaces

\[ K_k(A, v) = \text{span}\{v, Av, \ldots, A^{k-1}v\} \]

called the Krylov subspaces. The dimension of these subspaces is increasing up to an index \( d = d(A, v) \) called the degree of \( v \) with respect to \( A \), for which the maximal dimension is attained, and \( K_d(A, v) \) is invariant under multiplication with \( A \). Having an index \( k < d \), the Lanczos algorithm (Algorithm 1) constructs an orthonormal basis \( v_1, \ldots, v_{k+1} \) of the Krylov subspace \( K_{k+1}(A, v) \). The Lanczos vectors \( v_j \) satisfy the three-term recurrence

\[
\beta_{i+1} v_{i+1} = Av_i - \alpha_i v_i - \beta_i v_{i-1}, \quad i = 1, \ldots, k
\]

or, written in the matrix form,

\[
AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T
\]

where \( V_k = [v_1, \ldots, v_k] \), the vector \( e_k \) denotes the \( k \)th column of the identity matrix of an appropriate size (here of the size \( k \)), and \( T_k \) is the \( k \) by \( k \) symmetric tridiagonal matrix of the Lanczos coefficients,

\[
T_k = \begin{bmatrix}
\alpha_1 & \beta_2 & & \\
\beta_2 & \ddots & \ddots & \\
& \ddots & \ddots & \beta_k \\
& & \beta_k & \alpha_k
\end{bmatrix}
\]
Since the coefficients $\beta_j$ are positive, $T_k$ is a Jacobi matrix. The Lanczos algorithm works for any symmetric matrix, but if $A$ is positive definite, then $T_k$ is positive definite as well.

During computations in floating point arithmetic, rounding errors may have a significant influence on the computed results. In particular, the orthogonality among the Lanczos vectors is usually lost very quickly. In this paper we are interested in happy cases when this situation does not happen. In more detail, assuming that $d = n$ and considering the standard model of floating point arithmetic that satisfies the IEEE 754 standard, we look for a nonzero pattern of $A$ and $v$ such that no rounding errors appear during the computation of the Lanczos algorithm. The classical examples of arithmetics satisfying the IEEE 754 standard are the double precision (binary64), single precision (binary32), or half precision (binary16).

3. Exact computations in floating point arithmetic. Let $F$ denote the set of floating point numbers and let “$\circ$” is one of the basic operations (addition, subtraction, multiplication, division, square root). Suppose that $\alpha$ and $\beta$ are floating point numbers and that $\alpha \circ \beta$ is within the exponent range (otherwise we get overflow or underflow). Denote the floating point result by $\text{fl}(\alpha \circ \beta)$. Then, considering the standard model of floating point arithmetic, it holds that

$$\text{fl}(\alpha \circ \beta) = (\alpha \circ \beta)(1 + \delta), \quad |\delta| \leq u,$$

where $u$ is the unit roundoff. Obviously, if $\alpha \in F$, then

$$\text{fl}(1 * \alpha) = \alpha, \quad \text{fl}(-\alpha) = -\alpha, \quad \text{fl}(0 * \alpha) = 0, \quad \text{fl}(\alpha - \alpha) = 0, \quad \text{fl}(\alpha / \alpha) = 1.$$

It is easy to see that if $P \in F^{n \times n}$ is a permutation matrix, $v \in F^n$, $A \in F^{n \times n}$, then

$$\text{fl}(P^T P) = I, \quad \text{fl}(P v) = P v, \quad \text{fl}(P A) = P A, \quad \text{fl}(A \cdot P) = AP.$$

In the following lemma we show that if $\alpha \in F$ and if $\alpha^2$ is within the exponent range, then the square root of the second power of $\alpha$ is computed exactly; see also [2, Question 1.17].

**Lemma 3.1.** Consider the standard model of floating point arithmetic. Let $\alpha \in F$ be a floating point number such that $\alpha^2$ is within the exponent range. Then it holds that

$$|\alpha| = \text{fl}\left(\sqrt{\text{fl}(|\alpha|^2)}\right).$$

**Proof.** Assume without loss of generality that $\alpha \geq 0$, otherwise we replace $\alpha$ by $|\alpha|$ in the text below. For $\beta \equiv \text{fl}(\alpha^2)$ it holds that

$$\beta = \alpha^2(1 + \delta), \quad |\delta| \leq u,$$

and the exact square root of $\beta \in F$ is given by

$$\sqrt[3]{\beta} = \alpha \sqrt{1 + \delta} = \alpha \left(1 + \frac{\delta}{2} - \frac{\delta^2}{8} + \frac{\delta^3}{16} + O(\delta^4)\right) = \alpha \left(1 + \frac{\delta}{2} + O(u^2)\right),$$

where we have used the Taylor expansion of $\sqrt{1 + \delta}$.

The IEEE 754 standard of floating point arithmetic guarantees that $\text{fl}(\sqrt[3]{\beta})$ is the nearest floating point number to the exact value of $\sqrt[3]{\beta}$. Since $\alpha$ is a floating point number, the two nearest floating point numbers to $\alpha$ are given by $\alpha(1 \pm 2u)$, where $2u$ is the machine epsilon. In other words,

$$\alpha(1 - 2u), \, \alpha, \, \alpha(1 + 2u).$$
are three consecutive floating point numbers. Comparing (3.1) and (3.2), the nearest floating-point number to $\sqrt{\beta}$ is $\alpha$. \hfill $\blacksquare$

Considering a vector

\begin{equation}
    z = \alpha e_j, \quad \alpha \in \mathbb{F},
\end{equation}

such that $\alpha^2$ is within the exponent range, then the previous lemma shows that the Euclidean norm of $z$ is in the standard model of floating point arithmetic computed exactly. On the other hand, if $z$ is not a multiple of $e_j$, then, in general, one can expect that rounding errors occur. In other words, the only structure of $z$ that guarantees that no rounding errors occur during the computation of its Euclidean norm is the structure (3.3).

4. Lanczos algorithm in floating point arithmetic. On line 8 of Algorithm 1, the Euclidean norm of the vector $z$ is computed. To guarantee that the Lanczos algorithm computes exactly for any matrix and any starting vector having a given structure, the Lanczos vectors must necessarily be equal to the columns of the identity matrix (up to the sign); see (3.3) and the discussion herein. In particular, since the normalized starting vector is the first Lanczos vector $v_1$, it must hold that $v_1 = \pm e_j$ for some $j = 1, \ldots, n$. To simplify the notation, we define the signed permutation matrix as the permutation matrix with the entries $\pm 1$ instead of 1. In the following lemma we investigate the parametrization of all matrices $A$ and vectors $v$ with $d = n$ such that the exact Algorithm 1 produces Lanczos vectors having just one nonzero entry.

**Lemma 4.1.** Assuming exact arithmetic, Algorithm 1 applied to a symmetric $A \in \mathbb{R}^{n \times n}$ and $v \in \mathbb{R}^n$ such that $d = n$ produces Lanczos vectors equal to plus or minus columns of the identity matrix if and only if

\[ A = PTP^T, \quad v = \tilde{\beta}_1 P e_1, \]

with $P \in \mathbb{R}^{n \times n}$ being a signed permutation matrix, and $T \in \mathbb{R}^{n \times n}$ being a tridiagonal matrix of the form

\[ T = \begin{bmatrix}
    \tilde{\alpha}_1 & \tilde{\beta}_2 & & \\
    \tilde{\beta}_2 & \ddots & \ddots & \\
    & \ddots & \ddots & \tilde{\beta}_n \\
    & & \tilde{\beta}_n & \tilde{\alpha}_n
\end{bmatrix}, \]

where $\tilde{\beta}_j > 0$, $j = 1, \ldots, n$. Moreover, the tridiagonal matrix $T_n$ resulting from Algorithm 1 is equal to $T$.

**Proof.** Suppose first that the Lanczos vectors are equal to plus or minus columns of the identity matrix and that $d = n$, i.e., there is a signed permutation matrix $P$ such that $V_n = P$. Since $d = n$, we obtain in the last iteration of the Lanczos algorithm $AV_n = V_n T_n$ so that

\[ A = V_n T_n V_n^T = PTP^T, \]

where we set $T = T_n$. Moreover, $v_1 = P e_1$, and, therefore, the starting vector $v$ has to have the form $v = \tilde{\beta}_1 P e_1$ for some $\tilde{\beta}_1 > 0$.

On the other hand, suppose that $A = PTP^T$ and $v = \tilde{\beta}_1 P e_1$ for some signed permutation matrix $P$ and $\tilde{\beta}_1 > 0$. Applying the Lanczos algorithm to $A$ and $v$, we get

\begin{equation}
    AV_n = V_n T_n.
\end{equation}
The choice of $v$ ensures that the first column $v_1$ of $V_n$ is equal to the first column $p_1$ of $P$. Moreover, from the assumption on the structure of $A$ it follows

$$AP = PT.$$  

Comparing (4.1) and (4.2) and using the fact that $p_1 = v_1$, $P$ is orthogonal, and $T$ is Jacobi with positive off-diagonal entries, we obtain $T_n = T$ and $V_n = P$. \[ \square \]

In the following theorem we show that the structure of $A$ and $v$ introduced in Lemma 4.1 is sufficient for the Lanczos algorithm to compute exactly in the standard floating point arithmetic.

**Theorem 4.2.** Consider the standard model of floating point arithmetic. Let

$$A = PTP^T, \quad v = \tilde{\beta}_1 Pe_1,$$

where $P \in \mathbb{F}^{n \times n}$ is a signed permutation matrix, and $T \in \mathbb{F}^{n \times n}$ is tridiagonal of the form

$$T = \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_2 & \cdots & \cdots & \tilde{\beta}_n \\ \tilde{\beta}_2 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \tilde{\beta}_n & \cdots & \cdots & \cdots & \tilde{\alpha}_n \end{bmatrix},$$

with $\tilde{\beta}_j > 0$ and $\tilde{\beta}_j^2$ within the exponent range. Then Algorithm 1 applied to $A$ and $v$ computes exactly, i.e., no rounding errors appear during the computations. As a consequence, it holds $T_n = T$.

**Proof.** The proof is by induction. Let us denote by bar the results of the computations in floating point arithmetic. We start on lines 2 and 3 of Algorithm 1. It is easy to check that $\bar{v} = \text{fl}(\tilde{\beta}_1 Pe_1) = v$, $\bar{v}_0 = 0 = v_0$, $\tilde{\beta}_1 = \text{fl}(||v||) = \beta_1 = \beta_1$, and $\bar{v}_1 = \text{fl}(v/\beta_1) = v_1$ are computed exactly.

Define the vector $e_0 = 0$ and assume that for $1 \leq i \leq n - 1$ the vectors $v_j = Pe_j$, $j = 0, \ldots, i$, the coefficients $\alpha_j = \tilde{\alpha}_j$, $j = 1, \ldots, i - 1$, and $\beta_j = \tilde{\beta}_j$, $j = 1, \ldots, i$ are computed exactly. Using results of Section 3, the induction hypothesis, and observing that $\bar{w} = \text{fl}(\text{fl}(Ae_i)) = \beta_i e_i(1 - \beta_i e_i)$, we obtain on line 5

$$\bar{w} = P\text{fl} \left( \tilde{\beta}_i e_{i-1} + \tilde{\alpha}_i e_i + \tilde{\beta}_{i+1} e_{i+1} - \beta_i e_{i-1} \right) = P \left( \tilde{\alpha}_i e_i + \tilde{\beta}_{i+1} e_{i+1} \right) = w.$$

Further, on line 6 we get

$$\bar{\alpha}_i = \text{fl}(w^Tv_i) = \alpha_i = \alpha_i,$$

and, using $\text{fl}(\alpha_i v_i) = \alpha_i Pe_i$, on line 7

$$\bar{z} = \text{fl}(w - \text{fl}(\alpha_i v_i)) = P\text{fl} \left( \alpha_i e_i + \tilde{\beta}_{i+1} e_{i+1} - \alpha_i e_i \right) = \tilde{\beta}_{i+1} Pe_{i+1} = z.$$

Hence, $z = \bar{z}$ on line 8 is of the form (3.3), and

$$\tilde{\beta}_{i+1} = \text{fl}(||z||) = \beta_{i+1} = \beta_{i+1}$$

resulting on line 10 to $\bar{v}_{i+1} = \text{fl}(z/\beta_{i+1}) = Pe_{i+1} = v_{i+1}$. \[ \square \]
Note that the same results can be shown also for the classical Gram-Schmidt variant of Algorithm 1, where we first compute \( \alpha_k = v_k^T A v_k \), and then evaluate
\[
z = A v_k - \alpha_k v_k - \beta_k v_{k-1}.
\]

The results of Theorem 4.2 together with Lemma 4.1 indicate that the only nonzero structure of \( A \) and \( v \) that guarantees exact computations of the Lanczos algorithm in floating point arithmetic is given by (4.3). If \( A \) and \( v \) do not have special structure (4.3), the Lanczos algorithm can still compute exactly, but only in very special cases where the particular input data are chosen such that no rounding errors appear.

Theorem 4.2 and Lemma 4.1 can be analogously formulated for \( A \) and \( v \) with \( d < n \). In such case, instead of \( P \) and \( T \) we consider block diagonal matrices \( \tilde{P} \) and \( \tilde{T} \) of the form
\[
\tilde{P} = \begin{bmatrix} P & 0 \\ 0 & R_1 \end{bmatrix}, \quad \tilde{T} = \begin{bmatrix} T & 0 \\ 0 & R_2 \end{bmatrix},
\]
where \( P \) is a signed permutation matrix of size \( d \), \( T \) is a \( d \) by \( d \) tridiagonal matrix defined as in Theorem 4.2 and Lemma 4.1, and \( R_1, R_2 \) are arbitrary square matrices of size \( n-d \).

5. The conjugate gradient method. The results of the previous section motivate the question, whether analogous results can be obtained also for the conjugate gradient method that is closely related to the Lanczos algorithm.

Given a symmetric and positive definite (SPD) matrix \( A \in \mathbb{R}^{n \times n} \) and a right-hand side vector \( b \in \mathbb{R}^n \), we wish to solve a system of linear algebraic equations
\[
Ax = b
\]
using the conjugate gradient method (CG). Consider first the classical Hestenes and Stiefel variant of CG formulated in Algorithm 2.

Algorithm 2 Conjugate gradients

input \( A, b, x_0 \)
\[
r_0 = b - Ax_0
\]
\[
p_0 = r_0
\]
for \( k = 1, \ldots \) until convergence do
\[
\gamma_{k-1} = \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T A p_{k-1}}
\]
\[
x_k = x_{k-1} + \gamma_{k-1} p_{k-1}
\]
\[
r_k = r_{k-1} - \gamma_{k-1} A p_{k-1}
\]
\[
\delta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}
\]
\[
p_k = r_k + \delta_k p_{k-1}
\]
end for

It is well-known that the vectors and the coefficients generated by CG and the Lanczos algorithm are closely related. In particular, if Algorithm 1 is started with \( A \) and \( v = r_0 \), then, in exact arithmetic,
\[
(5.1) \quad v_{j+1} = (-1)^j \frac{r_j}{\| r_j \|}, \quad j = 0, \ldots, k.
\]

Let us recall that for \( A \) and \( v \) having the structure (4.3), the Lanczos vectors \( v_{j+1} \) are computed without any roundoff error, i.e., they remain exactly orthogonal during finite precision computations. Based on the relation (5.1) one could expect that the normalized CG
residual vectors, computed by Algorithm 2 started with the same input data, will also be close to orthogonal. We now perform a numerical experiment showing that the orthogonality among CG residuals can be lost in general.

We consider the Strakoš matrix [28], which is a diagonal matrix $\Lambda$ having the eigenvalues

$$\lambda_i = \lambda_1 + \frac{i - 1}{n - 1} (\lambda_n - \lambda_1) \rho^{n-i}, \quad i = 2, \ldots, n.$$  

In particular, we choose $n = 24$, $\lambda_1 = 10^{-3}$, $\lambda_n = 1$, $\rho = 0.7$ and define $v = [1, \ldots, 1]^T$. To ensure that the results will closely approximate the results of exact computations, we apply the Lanczos algorithm with double reorthogonalization to $\Lambda$ and $v$. In the last iteration we obtain the symmetric tridiagonal matrix $\bar{T}_n$ having (almost) the same spectrum as $\Lambda$.

Define $x_0 \equiv 0$, $A \equiv \bar{T}_n$ and $b \equiv e_1$ so that the input data $A$ and $b$ for the CG algorithm have the desired structure (4.3). Theorem 4.2 ensures that Algorithm 1 applied to $A$ and $b$ computes exactly. However, Figure 5.1 demonstrates that this is no more true for Algorithm 2.

In Figure 5.1 we plot the loss of orthogonality among the normalized residual vectors $\tilde{v}_{j+1} \equiv (-1)^j \frac{\bar{r}_j}{\|\bar{r}_j\|}, \quad j = 0, \ldots, k$, computed by Algorithm 2. The loss of orthogonality is measured using the quantity

$$\|\bar{V}_k^T \bar{V}_k - I\|_F,$$

where $\bar{V}_k = [\bar{v}_1, \ldots, \bar{v}_k]$. We observe that the orthogonality is lost quickly. As a consequence, the Hestenes and Stiefel version of CG (Algorithm 2) does not compute exactly and rounding errors influence significantly the performance of the algorithm.

We did not find a nonzero structure of the input data $A$ and $b$ such that Algorithm 2 computes (almost) exactly. Since the coefficients $\gamma_{k-1}$ and $\delta_k$ are ratios of two floating point numbers, it is very unlikely that such a structure exists. Nevertheless, we can use the knowledge about the exact computations of the Lanczos algorithm and the close relationship between both algorithms to develop an algorithmic version of CG that computes “almost exactly” for the input data having the structure (4.3). The idea is simply to compute the exact
Lanczos vectors and reconstruct the CG quantities from the Lanczos vectors. Sometimes, this
variant of the CG method is denoted as the cgLanczos algorithm; see [24].

By comparing the corresponding recurrences for computing the Lanczos vectors \( v_{j+1} \) (Algorithm 1) and the CG residual vectors \( r_j \) (Algorithm 2), and using (5.1) one can find the
relationship among the Lanczos and CG coefficients

\[
\beta_{k+1} = \sqrt{\frac{\delta_k}{\gamma_{k-1}}}, \quad \alpha_k = \frac{1}{\gamma_{k-1}} + \frac{\delta_{k-1}}{\gamma_{k-2}}, \quad \delta_0 = 0, \quad \gamma_{-1} = 1.
\]

Writing (5.3) in the matrix form we find out that CG computes implicitly the \( LDL^T \) factor-
ization of \( T_k \)

\[
T_k = \begin{bmatrix}
1 & \ell_1 & \cdots & \\
\ell_1 & 1 & \cdots & \\
& \vdots & \ddots & \\
& & & 1
\end{bmatrix}
\begin{bmatrix}
d_1 \\
\vdots \\
d_k
\end{bmatrix}
\begin{bmatrix}
1 & \ell_1 & \cdots & \\
\ell_1 & 1 & \cdots & \\
& \vdots & \ddots & \\
& & & 1
\end{bmatrix},
\]

where

\[
\ell_j = \sqrt{\delta_j}, \quad j = 1, \ldots, k-1, \quad \text{and} \quad d_j = \gamma_j^{-1}, \quad j = 1, \ldots, k,
\]

are easily expressible from the CG coefficients. Therefore, knowing \( T_k \), we can compute its
\( LDL^T \) factorization to reconstruct the CG coefficients. The factorization can be computed
using

\[
d_1 = \alpha_1, \quad \ell_j = \frac{\beta_{j+1}}{d_j}, \quad d_{j+1} = \alpha_{j+1} - \beta_{j+1} \ell_j, \quad j = 1, \ldots, k-1;
\]

see, e.g., [6, p.25].

Suppose now that the Lanczos vectors and coefficients are known. Assuming for simplic-
ity \( x_0 = 0 \), we would like to reconstruct the CG approximate solutions \( x_k \) from the Lanczos
process. It is well-known that

\[
x_k = V_k y_k, \quad T_k y_k = \|b\| e_1.
\]

In the special case of the input data having the structure (4.3) one can assume that \( T_k \in \mathbb{F}^{k \times k} \)
and \( \|b\| \in \mathbb{F} \) are computed exactly using Algorithm 1. If we are able to compute the solution
of the system \( T_k y_k = \|b\| e_1 \) exactly, then \( x_k = V_k y_k \) would be the exact CG approximation
since columns of \( V_k \) are just plus or minus columns of the identity matrix. However, in
general, the system \( T_k y_k = \|b\| e_1 \) has to be solved numerically and only the computed
solution \( \bar{y}_k \) is available.

Using [15, Theorem 9.14, p. 176], the numerical solution \( \bar{y}_k \) of the system with tridiago-
nal symmetric and positive definite \( T_k \) computed using the \( LDL^T \) factorization of \( T_k \) is the
exact solution of the perturbed problem

\[
(T_k + \Delta) \bar{y}_k = \|b\| e_1, \quad |\Delta| \leq 5u|T_k| = 5uT_k.
\]

Therefore,

\[
\bar{y}_k = (I + T_k^{-1} \Delta) \bar{y}_k.
\]

so that

\[
x_k - \bar{x}_k = V_k (y_k - \bar{y}_k) = V_k T_k^{-1} \Delta \bar{y}_k.
\]
Assuming that $5\kappa(A) < 1$, we get
$$
\|T_k^{-1}\Delta\| \leq 5\kappa(T_k) \leq 5\kappa(A) < 1.
$$
Hence, $I + T_k^{-1}\Delta$ is nonsingular and
$$
\| (I + T_k^{-1}\Delta)^{-1} \| \leq \frac{1}{1 - \|T_k^{-1}\Delta\|}.
$$
Finally, using $\|x_k\| = \|V_k y_k\| = \|y_k\|$ we obtain
$$
\frac{\|x_k - \bar{x}_k\|}{\|x_k\|} = \frac{\|T_k^{-1}\Delta\bar{y}_k\|}{\|y_k\|} = \frac{\|T_k^{-1}\Delta(I + T_k^{-1}\Delta)^{-1}y_k\|}{\|y_k\|} \leq \frac{5\kappa(T_k)}{1 - 5\kappa(A)} \leq \frac{5\kappa(A)}{1 - 5\kappa(A)}.
$$
The results are summarized in the following theorem.

**Theorem 5.1.** Let a symmetric and positive definite matrix $A$ and a vector $b$ have the structure (4.3). Suppose that $V_k$ and $T_k$ are computed using the Lanczos algorithm (Algorithm 1) applied to $A$ and $b$, and that the system $T_k y_k = \|b\| e_1$ is solved numerically using $LDL^T$ factorization giving the computed solution $\bar{y}_k$. Let $x_0 = 0$. Then, under the assumption $5\kappa(A) < 1$, the computed CG approximate solution $\bar{x}_k = V_k \bar{y}_k$, $k > 0$, satisfies

$$
(5.7) \quad \frac{\|x_k - \bar{x}_k\|}{\|x_k\|} \leq \frac{5\kappa(A)}{1 - 5\kappa(A)},
$$
where $x_k$ is the exact CG approximation.

The above results demonstrate that almost exact CG approximate solutions can be computed without reorthogonalization. Naturally, the above mentioned version of CG is not too efficient since it requires storing the Lanczos vectors $V_k$ and the matrix $T_k$. Below we derive a more efficient version of CG that preserves the above idea: first compute the Lanczos vectors and coefficients and then reconstruct the CG related quantities. Using

$$
\|r_k\| = \sqrt{\delta_k \delta_{k-1} \ldots \delta_1} \|r_0\| = \ell_1 \ldots \ell_k \|r_0\|
$$
we obtain

$$
(5.8) \quad r_k = (-1)^k \|r_k\| v_{k+1} \equiv (-1)^k \|r_0\| \ell_1 \ldots \ell_k v_{k+1},
$$
$$
(5.9) \quad p_k = r_k + \delta_k p_{k-1} = r_k + \ell_k^2 p_{k-1},
$$
$$
(5.10) \quad x_k = x_{k-1} + \gamma_{k-1} p_{k-1} = x_{k-1} + \frac{p_{k-1}}{d_k}.
$$
The final cgLanczos algorithm is given by Algorithm 3. For simplicity we choose $x_0 = 0$ so that $r_0 = b$. Note that the cgLanczos algorithm follows in a straightforward way from the results of [24, Section 4].

The Algorithm 3 has three parts marked out by brackets. First, the Lanczos vectors and coefficients are computed as in Algorithm 1. In the second part the algorithm computes the $LDL^T$ factorization via (5.3) and the last part computes the CG vectors $p_j$, $r_j$ and $x_j$ using (5.8)-(5.10). We can see immediately that if we apply Algorithm 3 to $A$ and $b$ having the
Algorithm 3 cgLanczos algorithm

Input $A, b$

$\beta_1 = 0, v_0 = 0, \ell_0 = 0, x_0 = 0$

$r_0 = b, p_0 = r_0,$

$\rho_0 = \|b\|$

$v_1 = b/\rho_0$

For $k = 1, \ldots$ do

$w = Av_k - \beta_k v_{k-1}$

$\alpha_k = w^T v_k$

$w = w - \alpha_k v_k$

$\beta_{k+1} = \|w\|$

$v_{k+1} = w/\beta_{k+1}$

$d_k = \alpha_k - \beta_k \ell_{k-1}$

$\ell_k = \frac{d_k}{\beta_k^2}$

$\rho_k = \ell_k \rho_{k-1}$

$x_k = x_{k-1} + \frac{p_{k-1}}{d_k}$

$r_k = (-1)^k \rho_k v_{k+1}$

$p_k = r_k + \ell_k^2 p_{k-1}$

end for

structure (4.3), the residual vectors are exactly orthogonal during finite precision computations as in the case of Algorithm 1. The computed coefficients $\bar{\ell}_j$ and $\bar{d}_j$ are almost exact in the sense

$T_k + \Delta = \bar{L}_k \bar{D}_k \bar{L}_k^T, \quad |\Delta| \leq 5uT_k,$

see [15, p. 174], where $\bar{L}_k$ and $\bar{D}_k$ are the computed factors of the $LDL^T$ factorization of $T_k$. Therefore, one can expect that the CG approximate solution $\bar{x}_k$ computed using Algorithm 3 will satisfy the relation (5.7).

For numerical demonstration we consider the same problem as at the beginning of this section, i.e., we consider $A$ and $b$ having the structure (4.3), that have been obtained from the Lanczos algorithm with double reorthogonalization applied to $A$ and $v$. However, instead of Hestenes and Stiefel version of CG (Algorithm 2) we apply the cgLanczos algorithm (Algorithm 3) to solve the system $Ax = b$ with $x_0 = 0$. It is clear that residuals must be exactly orthogonal. Hence, we measure the quality of results computed by Algorithm 3 using the $A$-orthogonality of the reconstructed direction vectors, and using the relative distance between the exact and the computed CG approximations.

In Figure 5.2 we plot the loss of $A$-orthogonality (dotted curve) among the normalized direction vectors

$\bar{p}_k = \frac{\tilde{p}_k}{\|\tilde{p}_k\|_A}$

computed by Algorithm 3. The loss of $A$-orthogonality is measured by the Frobenius norm of the matrix $P_k^T AP_k - I$, where $P_k = [\tilde{p}_0, \ldots, \tilde{p}_{k-1}]$. As expected, the loss of $A$-orthogonality is close to the machine precision level. Moreover, we also plot the quantity

$\frac{\|x_k - \bar{x}_k\|}{\|x_k\|}$

(dashed curve), where $\bar{x}_k$ were computed in double precision using Algorithm 3 and the exact approximations $x_k$ were computed using Algorithm 3 in extended precision arithmetic with
128 valid digits (Matlab’s vpa arithmetic). As expected and predicted by Theorem 5.1, the relative error is close to the machine precision level. Note that \( \kappa(A) = 10^{3} \).

6. Other algorithms. In Section 4 we parametrized matrices \( A \) and starting vectors \( v \) that guarantee exact computations of the Lanczos algorithm. In this section we demonstrate that the ideas of Section 4 can be generalized to other algorithms for computing bases of Krylov subspaces. In particular, if \( A \) is not symmetric, we can use the Arnoldi algorithm \([1]\) for computing the orthonormal basis, or the nonsymmetric Lanczos algorithm \([17]\) for computing the bi-orthogonal basis. When working with Krylov subspaces generated by symmetric matrices \( A^T A \) or \( AA^T \), one can consider the Golub-Kahan bidiagonalization \([5]\). The ideas can be further generalized to block Krylov subspaces method like the block-Lanczos \([7]\) or block-Arnoldi algorithms. We will show that there exists a nonzero structure of the input data that guarantees exact computations of the above mentioned algorithms. For each algorithm we define the index \( d \) that corresponds to the maximal dimension of the corresponding subspaces, and formulate the final results for \( d = n \). Nevertheless, all results can be generalized to the case \( d < n \) similarly as for the Lanczos algorithm; see Section 4.

6.1. Arnoldi algorithm. A natural generalization of the Lanczos algorithm for nonsymmetric matrices is the Arnoldi algorithm; see \([1]\). Given a square matrix \( A \in \mathbb{R}^{n \times n} \) and assuming \( k < d = d(A,v) \), the Arnoldi algorithm (Algorithm 4) computes an orthonormal basis \( v_1, \ldots, v_{k+1} \) of the Krylov subspace \( K_{k+1}(A,v) \). The computed vectors and coefficients satisfy

\[
AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^T,
\]

where \( V_k = [v_1, \ldots, v_k] \) and

\[
H_k = \begin{bmatrix}
  h_{1,1} & \cdots & \cdots & h_{1,k} \\
  h_{2,1} & \ddots & \ddots & \vdots \\
  \vdots & \ddots & \ddots & \vdots \\
  h_{k,k-1} & h_{k-1,k} & \cdots & h_{k,k}
\end{bmatrix}
\]

is upper Hessenberg with \( h_{j+1,j} > 0, j = 1, \ldots, k - 1 \). Note that if \( A \) symmetric, then \( H_k \) is symmetric and tridiagonal, and Algorithm 4 is equivalent to Algorithm 1.
Algorithm 4 Arnoldi algorithm

\begin{itemize}
  \item \textbf{input} \(A, v\)
  \item \(v_1 = v/\|v\|\)
  \item for \(j = 1, \ldots, k\) do
    \item \(w = Av_j\)
    \item for \(i = 1 : j\) do
      \item \(h_{i,j} = v_i^T w\)
      \item \(w = w - h_{i,j} v_i\)
    \item end for
    \item \(h_{j+1,j} = \|w\|\)
    \item \(v_{j+1} = \frac{w}{h_{j+1,j}}\)
  \item end for
\end{itemize}

Theorem 4.2 for the Lanczos algorithm can now be generalized in a straightforward way for the Arnoldi algorithm. We state the corresponding theorem without a proof.

**Theorem 6.1.** Consider the standard model of floating point arithmetic. Let

\[ A = PHP^T, \quad v = \tilde{h}_{1,0} Pe_1, \]

where \(P \in \mathbb{R}^{n \times n}\) is a signed permutation matrix and

\[ H = \begin{bmatrix}
\tilde{h}_{1,1} & \ldots & \ldots & \tilde{h}_{1,n} \\
\tilde{h}_{2,1} & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots \\
\tilde{h}_{n,n-1} & \tilde{h}_{n,n}
\end{bmatrix} \]

with \(\tilde{h}_{j+1,j} > 0\) and \(\tilde{h}_{j+1,j}^2\) within the exponent range, \(j = 0, \ldots, n - 1\). Then Algorithm 4 applied to \(A\) and \(v\) computes exactly. As a consequence, it holds that \(H_n = H\).

**6.2. Nonsymmetric Lanczos algorithm.** Given \(A \in \mathbb{R}^{n \times n}\) and \(v, w \in \mathbb{R}^n\), such that \(w^Tv \neq 0\), we denote

\[ d = \min(d(A, v), d(A^T, w)). \]

Assuming \(k < d\) and \(\beta_{i+1} \neq 0, i = 1, \ldots, k\), the nonsymmetric Lanczos algorithm [17] (Algorithm 5) computes two sets \(v_1, \ldots, v_{k+1}\) and \(w_1, \ldots, w_{k+1}\) of bi-orthogonal vectors. The vectors and coefficients generated by Algorithm 5 satisfy

\[ AV_k = V_k T_k + \gamma_{k+1} v_{k+1} e_k^T, \]
\[ A^T W_k = W_k T_k^T + \beta_{k+1} w_{k+1} e_k^T, \]
\[ W_k^T V_k = I, \]

where \(V_k = [v_1, \ldots, v_k] \in \mathbb{R}^{n \times k}\), \(W_k = [w_1, \ldots, w_k] \in \mathbb{R}^{n \times k}\), and

\[ T_k = \begin{bmatrix}
\alpha_1 & \beta_2 & \cdots & \cdots & \beta_k \\
\gamma_2 & \cdots & \cdots & \cdots & \gamma_k \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\cdots & \ddots & \ddots & \ddots & \cdots \\
\gamma_k & \cdots & \cdots & \cdots & \alpha_k
\end{bmatrix}. \]
Algorithm 5 nonsymmetric Lanczos algorithm

\textbf{Algorithm 5} nonsymmetric Lanczos algorithm

\textbf{input} $A$, $v$, $w$
\textbf{end for}

The nonsymmetric Lanczos algorithm is based on two three-term recurrences similar to the recurrence from the Lanczos algorithm. Using the same technique as for the Lanczos algorithm, we obtain an analogy of Theorem 4.2 that we present without a proof.

\textbf{Theorem 6.2.} Consider the standard model of floating point arithmetic. Let

$$ A = PTP^T, \quad v = \tilde{\gamma}_1 Pe_1, \quad w = \tilde{\beta}_1 Pe_1, $$

where $P \in \mathbb{F}^{n \times n}$ is a sign permutation matrix and $T \in \mathbb{F}^{n \times n}$ is tridiagonal of the form

$$ T = \begin{bmatrix}
\tilde{\alpha}_1 & \tilde{\beta}_2 \\
\tilde{\gamma}_2 & \ddots & \ddots \\
& \ddots & \ddots & \ddots \\
& & \tilde{\gamma}_n & \tilde{\beta}_n \\
& & & \tilde{\alpha}_n
\end{bmatrix}, $$

with $\tilde{\beta}_j \neq 0$, $\tilde{\gamma}_j > 0$ and $\tilde{\gamma}_j^2$ within the exponent range, $j = 1, \ldots, n$. Then Algorithm 5 applied to $A$, $v$ and $w$ computes exactly. As a consequence, it holds that $T_n = T$.

\textbf{6.3. Golub-Kahan bidiagonalization.} Let $A \in \mathbb{R}^{n \times m}$, $v \in \mathbb{R}^n$, and denote

$$ d = \min(d(AA^T, v), d(A^TA, A^Tv)). $$

Assuming $k < d$, the Golub-Kahan bidiagonalization [5] (Algorithm 6) generates two sets of orthonormal vectors $s_1, \ldots, s_{k+1}$ and $w_1, \ldots, w_k$. The coefficients $\gamma_i$ and $\delta_{i+1}$ that appear in Algorithm 6 are normalization coefficients.

\textbf{Algorithm 6} Golub-Kahan bidiagonalization

\textbf{Algorithm 6} Golub-Kahan bidiagonalization

\textbf{input} $A$, $v$
\textbf{end for}
Denoting $S_k = [s_1, \ldots, s_k] \in \mathbb{R}^{n \times k}$ and $W_k = [w_1, \ldots, w_k] \in \mathbb{R}^{m \times k}$, the vectors and coefficients generated by Algorithm 6 satisfy

\[
A^T S_k = W_k L_k^T,
\]

\[
AW_k = S_k L_k + s_{k+1} \delta_{k+1} e_k^T,
\]

where

\[
L_k = \begin{bmatrix}
\gamma_1 & \gamma_2 & & \\
\delta_2 & \gamma_2 & & \\
 & \ddots & \ddots & \\
 & & \delta_k & \gamma_k
\end{bmatrix}.
\]

Under the assumption $k < d$, the coefficients $\gamma_i$'s as well as $\delta_i$'s are positive, $i = 1, \ldots, k$.

It is well known that the Golub-Kahan bidiagonalization is closely related to the Lanczos algorithm. In more detail, the orthonormal columns of $S_k$ can be seen as the Lanczos vectors generated by $AA^T$ with the starting vector $v$. Similarly, $W_k$ contains the Lanczos vectors generated by $A^T A$ and $A^T v$. Therefore, it is not surprising that the results of Section 4 for the Lanczos algorithm can be analogously formulated also for the Golub-Kahan bidiagonalization. We present here (without a proof) an analogy of Theorem 4.2 formulated for $A \in \mathbb{F}^{n \times n}$.

**Theorem 6.3.** Consider the standard model of floating point arithmetic. Let

\[
A = PLP^T, \quad v = \tilde{\delta} P e_1,
\]

where $P \in \mathbb{F}^{n \times n}$ is a sign permutation matrix and $L \in \mathbb{F}^{n \times n}$ is bidiagonal of the form

\[
L = \begin{bmatrix}
\tilde{\gamma}_1 & & \\
\tilde{\delta}_2 & \tilde{\gamma}_2 & \\
& \ddots & \ddots \\
& & \tilde{\delta}_n & \tilde{\gamma}_n
\end{bmatrix},
\]

with $\tilde{\gamma}_j, \tilde{\delta}_j > 0$ and $\tilde{\gamma}_j^2, \tilde{\delta}_j^2$ within the exponent range. $j = 1, \ldots, n$. Then Algorithm 6 applied to $A$ and $v$ computes exactly. As a consequence, it holds that $L_n = L$.

**6.4. Block Lanczos algorithm.** The Lanczos algorithm has also an analogy for block matrices known as the block-Lanczos algorithm; see [7]. Given a block symmetric matrix $A \in \mathbb{R}^{n \times n}$ with $p$ by $p$ blocks, i.e., $n = mp$ for some $m \in \mathbb{N}$, and a block vector $U_1 \in \mathbb{R}^{n \times p}$, we can define a sequence of block Krylov subspaces

\[
K_k(A, U_1) = \text{colspan}\{U_1, AU_1, \ldots, A^{k-1}U_1\}
\]

and denote the maximal achievable dimension of these nested subspaces as $d = d(A, U_1)$.

Let $I$ denote the $p$ by $p$ identity matrix and let $0$ denote the $p$ by $p$ zero matrix. Let $U_1$ has orthonormal columns and $d = K_m(A, U_1) = n$. Assuming $k < m$, the block Lanczos algorithm (Algorithm 7) generates an orthonormal sequence of block vectors $U_i \in \mathbb{R}^{n \times p}$, i.e.,

\[
U_i^T U_j = \delta_{i,j} I \quad (\delta_{i,j} \text{ denotes Kronecker delta}),
\]

satisfying the relation

\[
A [U_1, \ldots, U_k] = [U_1, \ldots, U_k] T_k + R_{k+1} [0, \ldots, 0, I],
\]
Algorithm 7 block Lanczos algorithm

\begin{algorithm}
\textbf{input} $A \in \mathbb{R}^{n \times n}, U_1 \in \mathbb{R}^{n \times p}$ such that $U_1^TU_1 = I$
\quad $U_0 = U_1, B_1 = 0$
\quad $M_1 = U_1^T A U_1$
\quad \textbf{for} $i = 1, \ldots, k$ \textbf{do}
\quad \quad $R_{i+1} = AU_i - U_i M_i - U_{i-1} B_i^T$
\quad \quad $R_{i+1} = U_{i+1} B_{i+1}$ (QR factorization of $R_{i+1}$)
\quad \quad $M_{i+1} = U_{i+1}^T A U_{i+1}$
\quad \textbf{end for}
\end{algorithm}

where

\[
T_k = \begin{bmatrix}
M_1 & B_2^T \\
B_2 & \ddots & \ddots \\
& \ddots & \ddots & B_k^T \\
& & B_k & M_k
\end{bmatrix}
\]

is a block tridiagonal matrix. The blocks $M_j \in \mathbb{R}^{p \times p}, j = 1, \ldots, k$, are symmetric matrices and $B_{j+1} \in \mathbb{R}^{p \times p}, j = 1, \ldots, k-1$, are upper triangular matrices.

Further, we define the \textit{signed block permutation} matrix as a square block matrix with only one nonzero block in each block row and block column, where the nonzero blocks are sign permutation matrices. We now present an analogy of Theorem 4.2.

\textbf{Theorem 6.4.} Consider the standard model of floating point arithmetic. Let $n = mp$ for $n, m, p \in \mathbb{N}$, and let

\[ A = PTP^T, \quad U_1 = P \begin{bmatrix} I, 0, \ldots, 0 \end{bmatrix}^T, \]

where $P \in \mathbb{F}^{n \times n}$ is a signed block permutation matrix with blocks of size $p$, $I, 0 \in \mathbb{F}^{p \times p}$, and $T \in \mathbb{F}^{n \times n}$ is a block tridiagonal matrix of the form

\[
T = \begin{bmatrix}
\tilde{M}_1 & \tilde{B}_2^T \\
\tilde{B}_2 & \ddots & \ddots \\
& \ddots & \ddots & \tilde{B}_m^T \\
& & \tilde{B}_m & \tilde{M}_m
\end{bmatrix},
\]

where $\tilde{M}_i \in \mathbb{F}^{p \times p}$ are symmetric and $\tilde{B}_{i+1} \in \mathbb{F}^{p \times p}$ are upper triangular with positive entries on the diagonal. Assume that the QR factorization in Algorithm 7 is computed using the classical or modified Gram-Schmidt algorithm without any underflow or overflow. Then Algorithm 7 applied to $A$ and $U_1$ computes exactly. As a consequence, it holds that $T_m = T$.

\textbf{6.5. Linear solvers.} In the previous we discussed algorithms for computing bases of the corresponding subspaces. We have shown that if the input data have the prescribed nonzero structure, then the basis (block) vectors as well as the projected matrices (defined through the coefficients that appear in the algorithms) are computed exactly.

The general idea of linear solvers is to look for an approximate solution $x_k$ as a linear combination of the basis vectors. The coefficients of the linear combination are defined to be the solution of the projected problem. If the algorithm for computing the basis is exact, then
the projected problem is given exactly. To obtain \( x_k \), we have to solve the (exact) projected problem numerically. Hence, \( \tilde{x}_k \) is influenced only by rounding errors arising when solving the projected problem. Note that projected problems are solved using direct methods like Cholesky or QR factorizations, whose numerical behavior is well understood; see, e.g., [15]. In summary, one can expect that the computed approximate solution \( \tilde{x}_k \) is close to \( x_k \), if the projected problem is solved accurately.

To demonstrate the above general ideas, consider for example the Arnoldi algorithm, see Section 6.1, applied to \( A \) and \( v \) having the structure described by Theorem 6.1. For simplicity assume that \( \|v\| = 1 \). Then \( V_k \) as well as \[
H_{k+1,k} \equiv \begin{bmatrix} H_k \\ h_{k+1,k} e^T \end{bmatrix}
\]
are computed exactly. Starting with \( x_0 = 0 \), the GMRES method [26] constructs approximations \( x_k \) to the solution of \( Ax = v \) of the form

\[
x_k = V_k y_k, \quad y_k = \arg \min_y \|H_{k+1,k} y - v_1\|,
\]
where the least squares problem is solved numerically using the QR factorization. Denote the computed coordinate vector by \( \bar{y}_k \). Then the computed approximate solution \( \tilde{x}_k \) satisfies

\[
\|x_k - \tilde{x}_k\| = \|V_k y_k - V_k \bar{y}_k\| = \|y_k - \bar{y}_k\|.
\]

Similar consideration can be made for other linear solvers that are based on algorithms discussed in Sections 6.2–6.4.

7. Context and application of results. In this section we discuss the application of our results related to the Lanczos algorithm (Sections 4 and 5). Analogous considerations can be made also for other methods discussed in Section 6.

7.1. Various representatives of the original problem. Let \( M, N \in \mathbb{R}^{n \times n} \) be symmetric matrices, and let \( r, s \in \mathbb{R}^n \). We define an equivalence relation in the following way. We say that the problem represented by \((M, r)\) is equivalent to the problem \((N, s)\), if there is an orthogonal matrix \( Q \in \mathbb{R}^{n \times n} \) such that \( N = Q^T M Q \) and \( s = Q^T r \). Having defined the equivalence relation, one may split the set of all couples \((M, c)\) into equivalence classes.

In the case of the Lanczos algorithm, the original problem is represented by a symmetric matrix \( A \) and a unit norm starting vector \( v_1 \), so that all equivalent problems are of the form \((Q^T A Q, Q^T v_1)\). The equivalence of problems can also be seen via the distribution function \( \omega(\lambda) \) that corresponds to the original data. Let \( U \Lambda U^T \) be the spectral decomposition of \( A \), where \( U = [u_1, \ldots, u_n] \) is orthogonal and \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \). Assume for simplicity that the eigenvalues \( \lambda_i \) of \( A \) are distinct and increasingly ordered. For \( i = 1, \ldots, n \) denote

\[
\omega_i \equiv \left(u_i^T u_i\right)^2 \quad \text{so that} \quad \sum_{i=1}^n \omega_i = 1.
\]

The distribution function \( \omega(\lambda) \) that corresponds to \( A \) and \( v_1 \) is defined using

\[
\omega(\lambda) \equiv \begin{cases} 
0 & \text{for } \lambda < \lambda_1, \\
\sum_{j=1}^i \omega_j & \text{for } \lambda_i \leq \lambda < \lambda_{i+1}, \quad 1 \leq i \leq n - 1, \\
1 & \text{for } \lambda_n \leq \lambda;
\end{cases}
\]

see Figure 7.1.
If two problems share the same distribution function, then there exists an orthogonal matrix $Q$ that transforms one problem into the other, i.e., the problems are equivalent. All problems with the same distribution function form an equivalence class, and $(A, v_1)$ can be seen as a representative of this equivalence class. Another representative is $(\Lambda, w)$, where

$$w \equiv \left[ \omega_1^{1/2}, \ldots, \omega_n^{1/2} \right]^T,$$

or $(\Lambda, \tilde{w})$, where $\tilde{w} \equiv U^T v_1$. Finally, assuming for simplicity that $\omega_i \neq 0$ for $i = 1, \ldots, n$, it holds that $d = n$, and $(T_n, e_1)$ resulting from the exact Lanczos algorithm applied to $A$ and $v_1$ stands for yet another representative; see Figure 7.2. Therefore, any theoretical behaviour of the Lanczos algorithm (represented by the generated tridiagonal matrices $T_k$) can be observed for the initial data having the structure (4.3). In other words, concentrating on test problems having the structure (4.3) is not restrictive and covers any theoretical behaviour of the Lanczos algorithm.

The representative $(\Lambda, w)$ provides directly the key information about the distribution function. On the other hand, $(T_n, e_1)$ is the only representative that guarantees that the Lanczos algorithm (or the corresponding Stieltjes process, see, e.g., [9, 21]) will not be affected by rounding errors; see Theorem 4.2.

Assuming $d = n$ and having one of the representatives, one can ask how to compute the other representatives in a numerically reliable way. Starting from $(A, v_1)$, we can find $(T_n, e_1)$ using the Lanczos (or Arnoldi) algorithm with double reorthogonalization [12, 4]. If the double reorthogonalization is not used, the rounding errors can strongly influence the computations, and the computed $T_n$ can be completely different from the exact $T_n$. Instead of double reorthogonalization, one can alternatively use Householder reflections to transform $(A, v_1)$ to $(\tilde{T}, \tilde{v}_1)$, where $\tilde{T}$ is tridiagonal, and then Givens rotations to transform $\tilde{v}_1$ to $e_1$ while preserving the tridiagonal structure of the transformed matrix using the chasing the bulge strategy. In general, to compute the representative $(T_n, e_1)$ in a numerically reliable way, one has to store a dense matrix, and the cost of computations is then $O(n^3)$ flops.

Concerning the other two representatives, there exist numerically reliable transformations between $(T_n, e_1)$ and $(\Lambda, w)$ with the cost of $O(n^2)$ flops and low memory requirements. In more detail, starting from $(T_n, e_1)$, one can use the Golub-Welsh algorithm [8] to compute $(\Lambda, w)$. In the opposite way, having $(\Lambda, w)$, the $\epsilon k p w$ algorithm of Gragg and Harrod [9] or the pftoqd algorithm of Laurie [18] are capable to compute $(T_n, e_1)$ reliably.
7.2. Any theoretical behavior is observable also numerically. To investigate theoretical as well as numerical behaviour of Krylov subspace methods, it is crucial to ask convenient questions that help in understanding complicated phenomena. Here we discuss three questions of that kind.

An important question asked in literature, see, e.g., \cite{14, 27, 13, 11, 3, 19}, is about possible theoretical behaviour of the considered method. For example, in the case of the conjugate gradient method, one can prescribe any decreasing convergence curve for the $A$-norm of the error and, at the same time, any convergence curve for the residual norms (positive numbers), and then construct a symmetric positive definite matrix $A$ and a right hand side $b$ such that exact CG applied to $Ax = b$ generates the prescribed convergence curves; see \cite{14, 19}. In more detail, the CG coefficients $\delta_k$, see Algorithm 2, satisfy

$$\delta_k = \frac{\|r_k\|^2}{\|r_{k-1}\|^2}.$$ 

Therefore, if the residual norms are given, then $\delta_k$’s are known. Moreover, since

$$\|x - x_k\|^2_A = \gamma_k\|r_k\|^2 + \|x - x_{k+1}\|^2_A,$$ 

see \cite{14}, and residual norms as well $A$-norms of the error are prescribed, also $\gamma_k$’s are known. Finally, as discussed in Section 5, CG computes implicitly the $LDL^T$ factorization of the tridiagonal matrix $T_k$. Assuming again for simplicity that $d = n$, the coefficients $\delta_1, \ldots, \delta_{n-1}$ and $\gamma_0, \ldots, \gamma_{n-1}$ determine uniquely the tridiagonal matrix $T_n$. Defining $A = T_n$ and $b = \|r_0\|e_1$, we obtain a system of linear equations such that exact CG applied to $Ax = b$ generates the prescribed residual norms and $A$-norms of the error. For more details and the related discussion, see \cite{19}. Let us emphasize that the constructed matrix is a Jacobi matrix and that the right hand side vector is a multiple of $e_1$.

Another question that can help in understanding numerical behaviour of Krylov subspace methods is the following one. Can the observed numerical behaviour be interpreted as the behaviour of the exact algorithm applied to a problem that is, in some sense, close to the
original one? In other words, we would like to find a mathematical model of the results of finite precision computations of the considered algorithm. Note that the term “a problem close to the original one” can have different meanings. For example, it can be understood in the classical backward error sense, i.e., one can look for a small perturbation of the original data, or, as in the case of the Lanczos and CG algorithms, one can look for a small perturbation of the distribution function \( \omega(\lambda) \) discussed in Subsection 7.1. In particular, Greenbaum [10] showed that the results of the finite precision Lanczos algorithm can be interpreted as the results of the exact Lanczos algorithm applied to a larger problem with a matrix having clustered eigenvalues around the original eigenvalues of \( A \). The perturbed distribution function has larger support (clusters of eigenvalues) and the sum of weights that correspond to the \( i \)th cluster is equal to the original weight \( \omega_i \). Note that the larger matrix, used in [10] for simulating the behaviour of the finite precision Lanczos algorithm, was a Jacobi matrix, and that the starting vector was a multiple of \( e_1 \). Analogous results can be obtained also for CG, but here the exact CG algorithm applied to the model problem will not generate exactly the same convergence curves (the residual norms and the \( A \)-norms of the error) as the finite precision CG algorithm applied to the original data. However, it will generate their very close approximations; see [10].

We now comment on our results. We have shown that if the matrix \( A \) and the starting vector \( v \) have the structure described in (4.3), then the Lanczos algorithm computes exactly in the standard floating point arithmetic. Moreover, a variant of CG (Algorithm 3) applied to \( Ax = b \) where \( A \) and \( b \) have the structure (4.3), computes almost exactly. Hence, since the above mentioned questions lead to systems having the structure (4.3), our results allow to check the answers numerically and without reorthogonalization, even for large problems.

Moreover, results of this paper give the answer to the following question: Can any theoretical behavior of the Lanczos and CG algorithms be observed also numerically (up to the relative accuracy limited by machine precision), without using reorthogonalization or extended precision arithmetic? In more detail, the theoretical behaviour of the Lanczos algorithm is represented by the generated matrices \( T_k \). As discussed in Section 7.1, any theoretical behavior of the Lanczos algorithm can be observed for the representative \((T, e_1)\), where \( T \in \mathbb{R}^{n \times n} \) is a Jacobi matrix. The results of the exact Lanczos algorithm applied to \( T \) and \( e_1 \) are then represented by the leading principal submatrices of \( T \). Converting the matrix \( T \) into the considered floating point arithmetic we obtain \( \bar{T} = \text{fl}(T) \), and the data \((\bar{T}, e_1)\) have the structure (4.3). Therefore, the finite precision Lanczos algorithm applied to \( \bar{T} \) and \( e_1 \) computes exactly, i.e., it generates the leading principal submatrices \( \bar{T}_k \) of \( \bar{T} \), and it holds that \( \bar{T}_k = \text{fl}(T_k) \). In this sense, any theoretical behavior of the Lanczos algorithm represented by real matrices \( T_k \) can be observed also numerically. Using the results of Section 5, analogous conclusion holds also for CG implemented using Algorithm 3.

7.3. Theoretical study of (large) model problems. Numerical experiments studying theoretical behaviour of the CG and Lanczos algorithms, but also of other methods and algorithms mentioned in Section 6, are in general restricted to relatively small problems only. To be sure that the computed results agree with the exact results one either has to reorthogonalize or to use extended precision arithmetic. To reorthogonalize, all the basis vectors have to be stored, and memory requirements do not allow to handle large problems. When using extended precision arithmetic, one usually has to consider a huge number of valid digits leading to very slow computations even for small problems.

The results of this paper provide a new practical tool for the analysis of the theoretical as well as finite precision behaviour of the considered algorithms, including the analysis of the behaviour of error estimates, e.g., the error estimates of the \( A \)-norm of the error in CG. We can use this tool in the standard floating point arithmetic, without reorthogonalization, and
for potentially very large problems. We only have to be able to construct model problems having the desired properties and the prescribed nonzero structure. Then, the prescribed nonzero structure ensures that the finite precision computations are exact for the algorithms that compute the basis vectors, and almost exact for the corresponding linear solvers.

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