MINRES: From Negative Curvature Detection to Monotonicity Properties

Yang Liu∗ Fred Roosta†

June 14, 2022

Abstract
The conjugate gradient method (CG) has long been the workhorse for inner-iterations of second-order algorithms for large-scale nonconvex optimization. Prominent examples include line-search based algorithms, e.g., Newton-CG, and those based on a trust-region framework, e.g., CG-Steihaug. This is mainly thanks to CG’s several favorable properties, including certain monotonicity properties and its inherent ability to detect negative curvature directions, which can arise in nonconvex optimization. This is despite the fact that the iterative method-of-choice when it comes to real symmetric but potentially indefinite matrices is arguably the celebrated minimal residual (MINRES) method. However, limited understanding of similar properties implied by MINRES in such settings has restricted its applicability within nonconvex optimization algorithms. We establish several such nontrivial properties of MINRES, including certain useful monotonicity as well as an inherent ability to detect negative curvature directions. These properties allow MINRES to be considered as a potentially superior alternative to CG for all Newton-type nonconvex optimization algorithms that employ CG as their subproblem solver.

1 Introduction
Consider the linear least-squares problem
\[
\min_{x \in \mathbb{R}^d} \|Ax - b\|^2,
\]
(1)
where \(A \in \mathbb{R}^{d \times d}\) is a symmetric but potentially indefinite and/or singular matrix and \(b \in \mathbb{R}^d\). Clearly, (1) includes, as a special case, the symmetric linear system \(Ax = b\). Among many iterative algorithms designed for such a setting, e.g., [2, 10, 11, 19], the minimum residual method (MINRES), introduced in the seminal work of Paige and Saunders [19], is arguably the preferred Krylov subspace method. Even when \(A\) is positive definite, it has been shown that MINRES enjoys several advantageous properties that allow it to be considered a superior alternative to the primary workhorse, the conjugate gradient method (CG). For example, on positive definite system, it has been shown in [9] that, just like CG, not only does MINRES have monotonicity properties in terms of the iterate norms, but also both the Euclidean and the energy norms of the error are monotonic. However, in sharp contrast to CG, MINRES also provides monotonicity in the residual (and more general backward errors). In this light, when the stopping rule is based on the residual (or backward errors), [9] demonstrate that MINRES can often converge orders of magnitude faster than CG.

In the context of optimization of a twice continuously differentiable function \(f : \mathbb{R}^d \to \mathbb{R}\), subproblems of the form (1) arise often where \(A\) and \(b\) are related to the Hessian and gradient of \(f\), and \(x\) is a direction for updating the optimization iterate, e.g., Newton’s direction is given with \(A = \nabla^2 f(w)\) and \(b = -\nabla f(w)\). In such settings, the superior performance of MINRES over CG has further been verified in [15,20], where a variant of Newton’s method employing MINRES as inner-solver, called Newton-MR,
has been shown to greatly outperform the classical Newton-CG [17] for optimization of strongly convex problems.

Despite such theoretical and empirical observations, the application of MINRES as subproblem solver for nonconvex Newton-type optimization methods has been very limited; an exception is [20], where nonconvexity is limited to invex optimization problems. This is in sharp contrast to CG, which has historically been used to calculate the update direction within many line-search and trust-region variants of second-order nonconvex optimization algorithms [4, 17]. Beyond certain implied monotonicity properties, this is greatly thanks to CG’s ability to naturally detect available nonpositive curvature (NPC) directions, i.e., some \( v \in \mathbb{R}^d, v \neq 0 \), for which \( \langle v, Av \rangle \leq 0 \). Such directions provide a valuable tool within the optimization iterations to avoid entrapment in undesirable saddle points. In fact, beyond CG, all conjugate direction methods such as conjugate residual (CR) [22, 24] involve iterations that allow for ready access to NPC directions, when they arise. Such inherent ability has prompted researchers to design nonconvex Newton-type optimization algorithms, which leverage conjugate-direction methods as subproblem solvers and, by nontrivial use of NPC directions, come equipped with favorable convergence properties, e.g., [5,6,18,21,26,27].

However, due to complicated dynamics of its iterations, similar properties for MINRES have not been available. In this paper, we set out to shed more light on MINRES and its underlying properties when applied to symmetric but potentially indefinite and/or singular systems. In doing so, not only do we establish several desirable monotonicity properties of MINRES, which mimic and at times improve those of CG, but also we show that MINRES indeed comes equipped with natural ability to detect NPC directions. It is hoped that such properties pave the way for further adoption of MINRES, as a potentially superior alternative to CG, within the class of nonconvex Newton-type optimization algorithms.

The rest of the paper is organized as follows. We end this section by introducing our notation and definitions as well as highlighting our main contributions. In Section 2, we briefly review MINRES and all its ingredients. We then provide our theoretical analysis of the properties of MINRES in Section 3. This includes its inherent ability to detect NPC directions (Section 3.1) and several other useful properties such as monotonicity (Section 3.2). Conclusion and further thoughts are gathered in Section 5.

Notation and definitions

Throughout the paper, vectors and matrices are denoted by bold lower-case and bold upper-case letters, respectively, e.g., \( \mathbf{b} \) and \( \mathbf{A} \). We use regular lower-case letters to denote scalar constants, e.g., \( d \). For two real vectors \( \mathbf{v}, \mathbf{w} \), their inner-product is denoted by \( \langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^\top \mathbf{w} \). For a vector \( \mathbf{v} \), its Euclidean norm is denoted by \( \| \mathbf{v} \| \). The iteration counter for the main algorithm appears as a subscript. The zero vector is denoted by \( \mathbf{0} \), while \( e_j \) denotes the \( j \)th column of the identity matrix. The zero matrix is denoted by \( \mathbf{0} \), while the identity matrix of dimension \( k \times k \) is denoted by \( \mathbf{I}_k \). \( \mathbf{A} \succeq \mathbf{0} \) indicate that the matrix \( \mathbf{A} \) is positive semi-definite, while \( \mathbf{A} \succ \mathbf{0} \) denotes positive definiteness. Also, for a symmetric matrix \( \mathbf{A} \), we denote \( \| \mathbf{x} \|_\mathbf{A} = \mathbf{x}^\top \mathbf{A} \mathbf{x} \) (this is an abuse of notation since unless \( \mathbf{A} \succ \mathbf{0} \), this does not imply a norm). For any \( k \geq 1 \), \( \mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \text{Span}\{\mathbf{b}, \mathbf{A} \mathbf{b}, \ldots, \mathbf{A}^{k-1} \mathbf{b}\} \) denotes the Krylov subspace of degree \( k \) generated using \( \mathbf{b} \) and \( \mathbf{A} \). The residual vector at iteration \( k \) is denoted by \( \mathbf{r}_k = \mathbf{b} - \mathbf{A} \mathbf{x}_k \).

**Remark 1** (Initialization). For simplicity, we assume that \( \mathbf{x}_0 = \mathbf{0} \) and hence \( \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) = \mathcal{K}_k(\mathbf{A}, \mathbf{b}) \).

The arguments and derivations can be accordingly modified to account for a nonzero initialization.

Motivated by optimization applications where \( \mathbf{A} \) is typically the Hessian encoding the geometry of the optimization landscape, Definition 1 describes what we refer to as a nonpositive curvature direction. This simply amounts to any direction that lies in the eigenspace corresponding to the nonpositive eigenvalues of \( \mathbf{A} \).

**Definition 1** (Nonpositive Curvature Direction). Any \( \mathbf{v} \in \mathbb{R}^d, \mathbf{v} \neq 0 \) for which \( \langle \mathbf{v}, \mathbf{A} \mathbf{v} \rangle \leq 0 \) is called a nonpositive curvature direction.

Clearly, the interplay between \( \mathbf{A} \) and \( \mathbf{b} \) is a critical factor in the convergence of MINRES and many other iterative solvers. This interplay is entirely characterized by the notion of the grade of \( \mathbf{b} \) with respect to \( \mathbf{A} \) as given in Definition 2; see [22] for more details.
Definition 2. The grade of \( b \) with respect to \( A \) is the positive integer \( g \in \mathbb{N} \) such that
\[
\text{dir} (K_k(A, b)) = \begin{cases} 
  k, & k \leq g, \\
  g, & k > g.
\end{cases}
\]

Contributions

Our main results can be summarized informally as follows.

Contributions and Main Results (Informal)

Property (I) As part of the MINRES iterations for solving (1), one can readily track a certain quantity without any additional cost (NPC Condition (9)) to determine if a nonpositive curvature is available at iteration \( k \). In this case, \( r_{k-1} \) (the residual vector of the previous iteration) can be declared as such a direction (Theorem 1).

Property (II) Under a certain mild condition on the grade of \( b \) with respect to \( A \), when no nonpositive curvature direction is detected for all iterations, MINRES provides a certificate for positive semi-definiteness of \( A \) (Theorem 2). Moreover, as long as nonpositive curvature has not been detected, the MINRES iterates \( \{x_k\}_{k=1}^\infty \) have the following properties (Theorems 4 and 5), in addition to several others to be detailed later:

Property (III) \( \langle b, x_k \rangle > \langle x_k, Ax_k \rangle \).

Property (IV) \( m(x_k) < m(x_{k-1}) \), where \( m(x) \triangleq \langle x, Ax \rangle / 2 - \langle b, x \rangle \).

Property (V) \( \|x_k\| > \|x_{k-1}\| \).

Remark 2. Consider an unconstrained optimization problem \( \min_{w \in \mathbb{R}^d} f(x) \) with a twice continuously differentiable objective \( f : \mathbb{R}^d \rightarrow \mathbb{R} \), and let \( A = \nabla^2 f(w) \) and \( b = -\nabla f(w) \). Several observations can be immediately made to support our position in advocating the use of MINRES as a good subproblem solver within many Newton-type optimization algorithms.

- At iteration \( k \) of MINRES, the residual vector \( r_{k-1} \) and quadratic value \( \langle r_{k-1}, Ar_{k-1} \rangle \) are both readily available without additional computational cost (Lemma 1). **Property (I)** guarantees that if a NPC direction is available at iteration \( k \), we must have \( \langle r_{k-1}, Ar_{k-1} \rangle \leq 0 \). That is, \( r_{k-1} \) is one such direction that can be readily used within the optimization algorithm.

- Let \( f \) be a strongly convex function for which we have \( A > 0 \). The iterates of CG in this case can be defined as
\[
x_k = \text{arg min}_{x \in K_k(A, b)} \frac{1}{2} \langle x, Ax \rangle - \langle b, x \rangle.
\]
Since \( 0 \in K_k(A, b) \), the optimal value of the above quadratic must be nonpositive. This implies that \( \langle b, x_k \rangle \geq \langle x_k, Ax_k \rangle / 2 > 0 \). In other words, in Newton-CG applied to a strongly convex problem, all CG iterations amount to descent directions, i.e., \( \langle x_k, \nabla f(w) \rangle < 0 \), \( \forall k \).

From **Property (III)**, we see that not only does every iteration of MINRES amount to a descent direction, but also MINRES can produce a better direction in that the amount of descent can be greater than the equivalent direction obtained from CG.

- **Property (IV)** and **Property (V)** of CG are the main driving force for its widespread use within trust-region algorithms, e.g., CG-Steinhaug [4, 23]. Since MINRES also satisfies these properties, it can now be considered a viable alternative to CG for approximately solving the subproblems of the trust-region framework.
2 MINRES: Review

For the sake of completeness, we recall the MINRES algorithm in some detail and introduce further notation that is used as part of our results. More details can be found in the original work [19] and many textbooks on the topic, e.g., [1, 7, 11].

Recall that MINRES iterations, at a high level, can be written as

$$x_k = \arg \min_{x \in k_k(A,b)} \|b - Ax\|.$$  

At its core, MINRES involves three major ingredients, as depicted in Algorithm 1: Lanczos process, QR decomposition, and update of the iterate.

Lanczos process

With $v_1 = b/\|b\|$, recall that after $k$ iterations of the Lanczos process, and in the absence of round-off errors\(^1\), the Lanczos vectors form an orthogonal matrix $V_{k+1} = [v_1 \; v_2 \; \ldots \; v_{k+1}] \in \mathbb{R}^{d \times (k+1)}$, whose columns span $K_{k+1}(A, b)$, and satisfy

$$AV_k = V_{k+1} \tilde{T}_k,$$

where $\tilde{T}_k \in \mathbb{R}^{(k+1) \times k}$ is an upper Hessenberg matrix of the form

$$\tilde{T}_k = \begin{bmatrix} \alpha_1 & \beta_2 & \beta_3 \\ \beta_2 & \alpha_2 & \beta_3 \\ \beta_3 & \alpha_3 & \ddots & \ddots \\ \vdots & \ddots & \ddots & \beta_k \\ & \ddots & \ddots & \beta_k \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{bmatrix} \triangleq \begin{bmatrix} T_k \\ \beta_{k+1} e_k^T \end{bmatrix}.$$  

Subsequently, we get the three-term recursion

$$\mathbf{Av}_k = \beta_k v_{k-1} + \alpha_k v_k + \beta_{k+1} v_{k+1}, \quad k \geq 2.$$  

In this light, every iteration of MINRES requires exactly one matrix-vector product. If $x_k = V_k y_k$ for some $y_k \in \mathbb{R}^d$, the residual $r_k$ can be written as

$$r_k = b - Ax_k = b - AV_k y_k = b - V_{k+1} \tilde{T}_k y_k = V_{k+1}(\|b\| e_1 - \tilde{T}_k y_k).$$

This gives the well-known subproblems of MINRES as

$$\min_{y_k \in \mathbb{R}^d} \|\beta_1 e_1 - \tilde{T}_k y_k\|, \quad \beta_1 = \|b\|.$$  

Recall that the grade of $b$ with respect to $A$, i.e., $g$ in Definition 2, determines the maximum rank that the triangular matrix $T_k$ can achieve, namely $\max \{ \text{Rank}(T_k); k \geq 0 \} \leq g$, $1 \leq k \leq d$. It is also well-known that, in exact arithmetic, the Lanczos process encounters the “lucky breakdown” after exactly $g$ iterations, i.e., $\beta_{g+1} = 0$, in which case MINRES returns a solution to (1).

QR decomposition

Recall that (4) is solved using the QR factorization of $\tilde{T}_k$. Let $Q_k \tilde{T}_k = R_k$ be the full QR decomposition\(^2\) of $\tilde{T}_k$, where $Q_k \in \mathbb{R}^{(k+1) \times (k+1)}$ and $R_k \in \mathbb{R}^{(k+1) \times k}$. Typically, $Q_k$ is formed, implicitly, by the application of a series of $2 \times 2$ reflections to transform $\tilde{T}_k$ to the upper-triangular matrix $R_k$. Each

\(^1\)For our theoretical derivations here, we assume the absence of round-off errors. Of course, in practice, such errors will result in a loss of orthogonality in the vectors generated by the Lanczos process, which may be safely ignored in many applications. However, if strict orthogonality is required, it can be enforced by a reorthogonalization strategy.

\(^2\)For the sake of notational simplicity and to avoid overusing the “transpose” operator in the discussion that follows, we have given the full QR factorization of $T_k$ in a more unconventional way where the Q factor is on the left.
reflection affects only two rows of the matrix being triangularized. More specifically, two successive reflections can be compactly written by considering the elements of the matrix that are being affected:

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & c_{i-1} & s_{i-1} \\
0 & s_{i-1} & -c_{i-1}
\end{bmatrix}
\begin{bmatrix}
c_{i-2} & s_{i-2} & 0 \\
s_{i-2} & -c_{i-2} & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
\gamma^{(1)}_{i-2} & \delta^{(1)}_{i-1} & 0 \\
\beta^{(1)}_{i-1} & \alpha^{(1)}_{i-1} & \beta^{(1)}_i \\
0 & \beta^{(1)}_i & \alpha^{(1)}_i \beta^{(1)}_{i+1}
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 0 \\
0 & c_{i-1} & s_{i-1} \\
0 & s_{i-1} & -c_{i-1}
\end{bmatrix}
\begin{bmatrix}
\gamma^{(2)}_{i-2} & \delta^{(2)}_{i-1} & 0 \\
\beta^{(2)}_{i-1} & \epsilon^{(2)}_{i-1} & \beta^{(2)}_i \\
0 & \beta^{(2)}_i & \epsilon^{(2)}_i \beta^{(2)}_{i+1}
\end{bmatrix}
\]

where \(3 \leq i \leq k - 1\) and

\[
c_j = \frac{\gamma_j^{(1)}}{\gamma_j^{(2)}}, \quad s_j = \frac{\beta_j^{(2)}}{\gamma_j^{(2)}}, \quad \gamma_j^{(2)} = \sqrt{\gamma_j^{(1)}^2 + \beta_j^{(1)} \gamma_j^{(1)}} = c_j \gamma_j^{(1)} + s_j \beta_j^{(2)} + 1 \leq j \leq k. \tag{5}
\]

Here, the \(2 \times 2\) submatrix made of \(c_j\) and \(s_j\) is the special case of a Householder reflector in dimension two [25, p. 76].

Consequently, we can rewrite \(Q_k\) and \(\tilde{R}_k\) in block form as

\[
Q_k \tilde{T}_k = \tilde{R}_k \triangleq \begin{bmatrix} \tilde{R}_k & 0^T \end{bmatrix}, \quad \tilde{R}_k \triangleq \begin{bmatrix}
\epsilon_3 & \cdots & \epsilon_4 \\
\gamma_3 & \cdots & \gamma_4 \\
\cdots & \cdots & \cdots \\
\gamma_{k-1} & \cdots & \gamma_k
\end{bmatrix}
\]

\[
Q_k \triangleq Q_{k,k+1} \begin{bmatrix} Q_{k-1} & 0 \\ I_{k-1} & c_k & s_k \\ s_k & -c_k & 0 \\ 0 & 0 & 0
\end{bmatrix}
\]

In fact, the same series of transformations are simultaneously applied to \(\beta_1 e_1\) as

\[
Q_k \beta_1 e_1 = \begin{bmatrix}
c_1 & s_1 c_2 & \cdots & s_1 s_2 \cdots s_{k-1} c_k \\
s_1 c_2 & \epsilon_2 & \cdots & s_1 s_2 \cdots s_{k-1} s_k
\end{bmatrix}
\triangleq \begin{bmatrix} \tau_1 & 0 \\ 0 & \tau_2 \\ \vdots & \vdots \\ 0 & \tau_k \\ \tau_k & \phi_k \end{bmatrix}
\triangleq \begin{bmatrix} t_k \\ \phi_k \end{bmatrix}
\]

With these quantities available, we can solve (4) by noting that

\[
\min_{y_k \in \mathbb{R}^k} ||r_k|| = \min_{y_k \in \mathbb{R}^k} ||\beta_1 e_1 - T_k y_k|| = \min_{y_k \in \mathbb{R}^k} ||Q_k \beta_1 e_1 - Q_k \tilde{T}_k y_k|| = \min_{y_k \in \mathbb{R}^k} \left\| \begin{bmatrix} t_k \\ \phi_k \end{bmatrix} - \begin{bmatrix} \tilde{R}_k \\ 0^T \end{bmatrix} y_k \right\|,
\]

so that \(\tilde{R}_k y_k = t_k\) and \(||r_k|| = \phi_k\) (note that, by construction, \(\phi_k\) remains non-negative throughout the iterations.) We also trivially have \(\phi_0 = \beta_1 = ||b||\).

**Updates**

Suppose \(k < g\) and define \(D_k\) from the lower triangular system \(R_0^T D_k = V_k^T\). Now, letting \(V_k = [V_{k-1} \mid v_k]\) and using the fact that \(R_k\) is upper-triangular, we get the recursion \(D_k = [D_{k-1} \mid d_k]\) for some vector \(d_k\). As a result, using \(R_k y_k = t_k\), one can update the iterate as

\[
x_k = V_k y_k = D_k R_k y_k = D_k t_k = [D_{k-1} \mid d_k] \begin{bmatrix} t_{k-1} \\ \tau_k \end{bmatrix} = x_{k-1} + \tau_k d_k.
\]
Furthermore, from $V_k = D_k R_k$, i.e.,

$$
[v_1 \ v_2 \ \ldots \ \ v_k] = [d_1 \ d_2 \ \ldots \ d_k]
$$

we get the following relationship for computing $v_k$ as

$$
v_k = \epsilon_k d_k - 2 + \delta_k^{(2)} d_{k-1} + \gamma_k^{(2)} d_k.
$$

All of the above steps constitute MINRES algorithm, which is given in Algorithm 1. For more details, see [1,2,3,7,9,11,19].

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**Algorithm 1 MINRES with Built-in NPC Detection**

**Input:** The matrix $A$, the right hand side vector $b$,

$\beta_1 = ||b||$, $r_0 = b$, $v_1 = b/\beta_1$, $v_0 = x_0 = d_0 = d_{-1} = 0$, $c_0 = -1$, $s_0 = 0$, $\phi_0 = \tau_0 = \beta_1$, $\delta_1^{(1)} = 0$, $k = 1$,

while True do

$p_k = Av_k$, $\alpha_k = v_k^T p_k$, $p_k = p_k - \beta_k v_{k-1}$, $p_k = p_k - \alpha_k v_k$, $\beta_{k+1} = ||p_k||$,

$\delta_k^{(2)} = c_{k-1} \delta_k^{(1)} + s_{k-1} \alpha_k$, $\gamma_k^{(1)} = s_{k-1} \delta_k^{(1)} - c_{k-1} \alpha_k$, $c_{k+1} = s_{k-1} \beta_{k+1}$, $\delta_{k+1}^{(1)} = -c_{k-1} \beta_{k+1}$,

if $c_{k-1} \gamma_k^{(1)} \geq 0$ then 

return $r_{k-1}$ as a NPC direction (NB: this is an optional return; see Remark 3),

end if

$\gamma_k^{(2)} = \sqrt{(\gamma_k^{(1)})^2 + \beta_{k+1}^2}$,

if $\gamma_k^{(2)} \neq 0$ then

$c_k = \gamma_k^{(1)}/\gamma_k^{(2)}$, $s_k = \beta_{k+1}/\gamma_k^{(2)}$, $\tau_k = c_k \phi_{k-1}$, $\phi_k = s_k \phi_{k-1}$,

$d_k = (v_k - \delta_k^{(2)} d_{k-1} - \epsilon_k d_{k-2})/\gamma_k^{(2)}$, $x_k = x_{k-1} + \tau_k d_k$,

if $\beta_{k+1} \neq 0$ then

$v_{k+1} = p_k/\beta_{k+1}$, $r_k = s_k^2 r_{k-1} - \phi_k c_k v_{k+1}$,

else

$r_k = 0$,

return $x_k$ as a solution to (1),

end if

else

$c_k = 0$, $s_k = 1$, $\tau_k = 0$, $\phi_k = \phi_{k-1}$, $r_k = r_{k-1}$, $x_k = x_{k-1}$,

return $x_k$ as a solution to (1),

end if

$k \leftarrow k + 1$,

end while

**Output:** A solution to (1) or a NPC direction.
Remark 3. Algorithm 1 is depicted such that the iterations are terminated when an NPC direction is detected. However, depending on the application, one may choose to continue the MINRES iterations to additionally find a solution, or a suitable approximation, to (1). In other words, while the detection of NPC direction is a feature that can be leveraged in many applications, it does not necessarily imply a termination to the MINRES iterations.

3 MINRES: Main properties

In this section, we provide several useful properties of MINRES when applied to symmetric but potentially indefinite and/or singular systems. These include its natural ability to detect NPC directions (Section 3.1) as well as many monotonicity properties (Section 3.2).

3.1 Nonpositive curvature detection

First, we show that MINRES comes naturally equipped with the ability to detect nonpositive curvature. More specifically, we show that whenever a certain readily verifiable condition within MINRES iteration holds, the residual of the previous iteration is one such direction.

Certificate of positive-definiteness of \( T_k \)

Since \( \mathbf{r}_{k-1} \in K_k(\mathbf{A}, \mathbf{b}) \), we can write \( \mathbf{r}_{k-1} = \mathbf{V}_k \mathbf{z} \) for some \( \mathbf{z} \in \mathbb{R}^k \) and \( \mathbf{V}_k \in \mathbb{R}^{d \times k} \) in (2). For \( \mathbf{r}_{k-1} \) to be a direction of nonpositive curvature, we must have \( \mathbf{r}_{k-1}^\top \mathbf{A} \mathbf{r}_{k-1} = \mathbf{z}^\top T_k \mathbf{z} \leq 0 \), i.e., we must have \( T_k \not\succ 0 \). We show that the converse also holds (Theorem 1). In other words, as soon as \( T_k \not\succ 0 \) within MINRES iterations, we must have \( \mathbf{r}_{k-1}^\top \mathbf{A} \mathbf{r}_{k-1} \leq 0 \). This amounts to showing that the sequence \( \{\mathbf{r}_{i-1}^\top \mathbf{A} \mathbf{r}_{i-1}; i = 1, \ldots, k\} \) provides a built-in certificate of positive-definiteness for \( T_k \).

We first show that \( \mathbf{r}_{i-1}^\top \mathbf{A} \mathbf{r}_{i-1} \) can be computed without additional matrix-vector products. Indeed, among other useful relations, Lemma 1 gives an equivalent expression for \( \mathbf{r}_{i-1}^\top \mathbf{A} \mathbf{r}_{i-1} \) that can be readily computed using scalar operations.

Lemma 1. Let \( g \) be the grade of \( \mathbf{b} \) with respect to \( \mathbf{A} \) as in Definition 2. We have

\[
x_i^\top \mathbf{A} \mathbf{r}_k = 0, \quad 1 \leq i \leq k \leq g,
\]

\[
\mathbf{r}_i^\top \mathbf{A} \mathbf{r}_k = 0, \quad 1 \leq i \leq g, \quad 1 \leq k \leq g, \quad i \neq k,
\]

\[
\mathbf{r}_{k-1}^\top \mathbf{A} \mathbf{r}_{k-1} = -\phi_{k-1}^2 c_{k-1} \gamma_k^{(1)}, \quad 1 \leq k \leq g,
\]

\[
\mathbf{r}_i^\top \mathbf{b} = \|\mathbf{r}_i\|^2, \quad 1 \leq k \leq g.
\]

Proof. First, recall that \( \mathbf{x}_0 = 0 \) implies \( \mathbf{x}_i \in K_i(\mathbf{A}, \mathbf{b}), \ i \leq k \). From Petrov–Galerkin conditions, we also have \( \mathbf{r}_k \perp \mathbf{A} K_k(\mathbf{A}, \mathbf{b}), \) which with \( \mathbf{A} \) real symmetric implies (7a). Now let \( i < k \), for which we have \( \mathbf{r}_i \in K_i(\mathbf{A}, \mathbf{b}) \). From \( \mathbf{A} \mathbf{r}_i \perp K_i(\mathbf{A}, \mathbf{b}) \), we get \( \mathbf{r}_i^\top \mathbf{A} \mathbf{r}_k = 0 \) for \( i < k \). From the symmetry of \( \mathbf{A} \), we get \( \mathbf{r}_i^\top \mathbf{A} \mathbf{r}_k = 0 \) for all \( i \neq j \), which gives (7b). Now, from [2,3] we know that in MINRES, \( \mathbf{r}_k \) and \( \mathbf{A} \mathbf{r}_k \) satisfy

\[
\mathbf{r}_k = s_k^2 \mathbf{r}_{k-1} - \phi_k c_k \mathbf{v}_{k+1}, \quad \mathbf{A} \mathbf{r}_k = \phi_k (\gamma_k^{(1)} \mathbf{v}_k + \delta_k^{(1)} \mathbf{v}_{k+1}).
\]

Noting that \( \mathbf{r}_{k-2} \perp \{\mathbf{v}_k, \mathbf{v}_{k+1}\} \), and \( \mathbf{v}_k \perp \mathbf{v}_{k+1}, \) we have

\[
\mathbf{r}_{k-1}^\top \mathbf{A} \mathbf{r}_{k-1} = (s_{k-1}^2 \mathbf{r}_{k-2} - \phi_{k-1} c_{k-1} \mathbf{v}_k)^\top (\phi_{k-1} (\gamma_k^{(1)} \mathbf{v}_k + \delta_k^{(1)} \mathbf{v}_{k+1})) = -\phi_{k-1}^2 c_{k-1} \gamma_k^{(1)},
\]

which gives (7c). Finally, from (7a) we get

\[
\mathbf{r}_i^\top \mathbf{b} = \mathbf{r}_i^\top (\mathbf{r}_k + \mathbf{A} \mathbf{x}_k) = \|\mathbf{r}_k\|^2,
\]

which yields (7d). \( \square \)
Theorem 1 states that if \( \gamma_k^{(1)} \geq 0 \), then \( r_{k-1} \) is a NPC direction for \( A \), i.e.,
\[
\frac{\langle r_{k-1}, Ar_{k-1} \rangle}{\|r_{k-1}\|^2} = -c_{k-1}\gamma_k^{(1)} \leq 0.
\]

Consider any \( \ell \leq g \). Since \( \text{Span}\{r_0, \ldots, r_{\ell-1}\} \subseteq K_\ell(A, b) = \text{Range}(V_{k}) \), we have \( r_{\ell-1} = V_{k}y \) for some \( y \in \mathbb{R}^k \). From \( T_{k} = V_{k}^\dagger AV_{k} \), it follows that \( r_{\ell-1}^T Ar_{k-1} = y^T T_{k} y \). As a result, if \( T_{k} > 0 \), then (7c) implies that the NPC condition (9) does not hold for any \( k \leq \ell \). In other words, if \( T_{k} > 0 \), then \( c_{k-1}\gamma_k^{(1)} < 0 \), \( \forall 1 \leq k \leq \ell \). Theorem 1 below provides a converse to this. In particular, it states that as soon as \( T_{k} \neq 0 \), the NPC condition (9) holds and \( r_{k-1} \) is identified as a NPC direction. That is, Theorem 1 states that if \( c_{k-1}\gamma_k^{(1)} < 0 \), \( \forall 1 \leq k \leq \ell \), then we must have \( T_{k} > 0 \).

\[\text{Remark 4 (NPC Condition). From (7c), we see that if} \]
\[c_{k-1}\gamma_k^{(1)} \geq 0, \]
then \( r_{k-1} \) is a NPC direction for \( A \), i.e.,
\[
\frac{\langle r_{k-1}, Ar_{k-1} \rangle}{\|r_{k-1}\|^2} = -c_{k-1}\gamma_k^{(1)} \leq 0.
\]

\[\text{Theorem 1 (Certificate for } T_{k} > 0\text{). Suppose } \ell \leq g \text{ where } g \text{ is the grade of } b \text{ with respect to } A \text{ as in Definition 2. If } T_{k} \neq 0 \text{, then the NPC condition (9) holds for some } k \leq \ell. \text{ In particular, if } k \leq g \text{ is the first iteration where } T_{k} \neq 0 \text{, then the NPC condition (9) holds.}\]

**Proof.** Suppose \( T_{\ell} \neq 0 \). We first note that \( k \leq g \) implies that \( r_{k-1} \neq 0 \), which in turn gives \( \phi_{k-1} \neq 0 \). From the properties of the Krylov subspace, we have \( \text{Span}\{r_0, \ldots, r_{\ell-1}\} \subseteq K_{\ell}(A, b) \). We now consider two cases.

(i) Let’s first consider the case where \( \text{Span}\{r_0, \ldots, r_{\ell-1}\} = K_{\ell}(A, b) \). Suppose for any nonzero \( z \in K_{\ell}(A, b) \), we have \( \langle z, Az \rangle > 0 \). Consequently, for any nonzero \( w \in \mathbb{R}^\ell \), we can let \( z = V_{\ell} w \in K_{\ell}(A, b) \) and have
\[
w^T T_{\ell} w = w^T V_{\ell}^\dagger A V_{\ell} w = z^T Az > 0.
\]
However, this implies that \( T_{\ell} > 0 \), which contradicts the assumption on \( T_{\ell} \). Hence, there must exists nonzero \( z \in K_{\ell}(A, b) \) for which \( z^T Az \leq 0 \). Let \( \xi_1, \ldots, \xi_\ell \) be scalars such that
\[
z = \sum_{k=1}^{\ell} \xi_k r_{k-1}.
\]
Suppose \( r_{\ell-1}^T Ar_{k-1} > 0 \) for all \( 1 \leq k \leq \ell \). Then by (7b), we have
\[
0 \geq z^T Az = \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \xi_i \xi_j r_{i-1}^T Ar_{j-1} = \sum_{k=1}^{\ell} \xi_k^2 r_{k-1}^T Ar_{k-1} > 0,
\]
which is a contradiction. Hence, we must have \( r_{\ell-1}^T Ar_{k-1} \leq 0 \) for some \( 1 \leq k \leq \ell \), i.e., the NPC condition (9) holds for some \( k \leq \ell \). In particular, if \( k \) is the first iteration where \( T_{k} \neq 0 \), we must in fact have \( r_{\ell-1}^T Ar_{k-1} \leq 0 \). In other words, as soon as \( T_{k} \) contains a nonpositive eigenvalue, the NPC condition (9) holds and hence the vector \( r_{k-1} \) is a nonpositive curvature direction.

(ii) Now suppose \( \text{Span}\{r_0, \ldots, r_{\ell-1}\} \subseteq K_{\ell}(A, b) \). Suppose \( k \leq \ell \) is the first iteration where the additional residual vector has not increased the Krylov space’s dimension, i.e., \( \text{Span}\{r_0, \ldots, r_{k-1}\} = K_{k-1}(A, b) \). In this case, since \( \text{Span}\{r_{k-2}, r_{k-1}\} \perp v_k \), by (8) we must have \( \phi_{k-1} r_{k-1} = 0 \), i.e., \( r_{k-1} = s_{k-1} r_{k-2} \). Since \( \phi_{k-1} \neq 0 \), we can only have \( c_{k-1} = 0 \) and \( s_{k-1} = 1 \), i.e., \( r_{k-1} = r_{k-2} \). Hence, by (7c), we get
\[
r_{k-2}^T Ar_{k-1} = r_{k-2}^T Ar_{k-2} = 0,
\]
which implies that both \( r_{k-1} \) and \( r_{k-2} \) are nonpositive curvature directions (this also implies that \( T_{k-1} \neq 0 \)). In fact, since \( \text{Span}\{r_0, \ldots, r_{k-2}\} = K_{k-1}(A, b) \), based on the discussion of the previous case, having \( r_{k-2}^T Ar_{k-2} = 0 \) implies that we should have already detected nonpositive curvature in the previous iteration.
It is possible to show that if $A \succeq 0$, then for any $1 \leq k \leq g - 1$, we have $r_{k+1}^i A r_{k+1} > 0$ and $T_k > 0$; see Lemma 2 below. More generally, however, for any real symmetric but not necessarily PSD matrix $A$, Theorem 1 implies that by keeping track of the NPC condition (9), if $r_{k+1}^i A r_{k+1} > 0$ for all $1 \leq i \leq k \leq g$, then $T_k > 0$. In other words, MINRES has a built-in mechanism to provide a certificate of positive definiteness (or lack thereof) for $T_k$.

Certificate for $A \succeq 0$

A natural question to ask is whether it is possible to provide a similar certificate for $A$ from within MINRES iterations? The question arises because, as part of the Lanczos process, one expects to see tight connections between the spectral properties of $A$ and $T_k$. For example, when $A > 0$, we trivially have $T_k > 0$, $1 \leq k \leq g$. In fact, having $A \succeq 0$ implies positive definiteness of $T_k$ for $1 \leq k \leq g - 1$.

Lemma 2. Suppose $A \succeq 0$ and let $g$ be the grade of $b$ with respect to $A$ as in Definition 2. The following statements hold.

(i) $T_k > 0$, $1 \leq k \leq g - 1$.
(ii) If $b \in \text{Range}(A)$, then $T_g > 0$.
(iii) If $b \notin \text{Range}(A)$, then $T_g \succeq 0$ is singular, $\gamma_g^{(2)} = 0$, and $r_{g-1}$ is a zero curvature direction.

Proof. From $T_k = V_k^i A V_k$ and $A \succeq 0$, it follows that $T_k \succeq 0$, $1 \leq k \leq g$. By the Sturm Sequence Property and the strict interlacing result [11, Theorem 8.4.1], the smallest eigenvalue of $T_i$ decreases to zero monotonically with $k$. As a result, only $T_g$ can potentially be singular in which case it will have exactly one zero eigenvalue. In other words, we must always have $T_k > 0$, $1 \leq k \leq g - 1$.

Now, if $b \in \text{Range}(A)$, then by [12, Property J2, p. 247], we know that $T_g > 0$. Otherwise, from [2, Theorem 3.2], it follows that $T_g$ is singular and $\gamma_g^{(1)} = 0$. Hence, by (7c), we have $r_{g-1}^i A r_{g-1} = 0$. In other words, $r_{g-1}$ is a zero curvature direction. Furthermore, since $\beta_{g+1} = 0$, we also get $\gamma_g^{(2)} = 0$ by (5).

From Lemma 2, it follows that when $A \succeq 0$, we have $T_k > 0$, $1 \leq k \leq g - 1$, and $T_g \succeq 0$ (if $b \in \text{Range}(A)$, we actually have $T_g > 0$). Theorem 2 below provides somewhat of a converse to this. More specifically, Theorem 2 shows that, under a certain condition on $g$, having $T_k > 0$, $1 \leq k \leq g$, provides a certificate for $A \succeq 0$. As a result, Theorem 2 shows that MINRES comes equipped with an inherent ability to provide a certificate of positive semi-definiteness for $A$. This, just like the case for $T_k$, can be done by tracking the NPC condition (9). In doing so, however, one has to also take into account the interplay of $A$ and $b$ as it relates to $g$, i.e., the grade of $b$ with respect to $A$ (Definition 2). Indeed, consider the case where $A$ is indefinite, but $b$ is an eigenvector corresponding to one of its positive eigenvalues. In this case, since $g = 1$, MINRES terminates after only one iteration and the negative spectrum of $A$ is never explored. To avoid such situations, we need $b$ to have a non-zero projection on the eigenspace corresponding to each eigenvalue of $A$, which is equivalent to $g$ being equal to the number of distinct eigenvalues of $A$.

Theorem 2 (Certificate for $A \succeq 0$). Assume $g$ equals the number of distinct eigenvalues of $A$, where $g$ is the grade of $b$ with respect to $A$ as in Definition 2. If $A \not\succeq 0$, then $T_k \not\succeq 0$ for some $k \leq g$, and hence the NPC condition (9) holds for some $k \leq g$.

Proof. Suppose $A \not\succeq 0$. If $k \leq g$ is the first iteration such that $T_k \not\succeq 0$, then by Theorem 1, we have that the NPC condition (9) holds. Now suppose, for all $k \leq g$, we always have $T_k \succeq 0$. In this case, in particular, we have $T_g = V_g^i A V_g \succeq 0$. Recall that the assumption on $g$ is equivalent to $b$ having a non-zero projection on the eigenspace corresponding to each eigenvalue of $A$. Hence, using a very similar line of reasoning as in the proof of [1, Theorem 2.6.2], we can show that $\text{Range}(V_g)$ contains an eigenvector corresponding to a negative eigenvalue of $A$. Let $v$ be such an eigenvector, so we get $\langle v, Av \rangle < 0$. Since $v \in \text{Range}(V_g)$, we can write $v = V_g w$ for some $w \in \mathbb{R}^k$. Now, it follows that

$$w^i T_g w = w^i V_g^i A V_g w = v^i Av < 0,$$
which contradicts having \( T_g \succ 0 \). Hence, we must have \( T_g \prec 0 \), which by Theorem 1 implies that the NPC condition (9) holds with \( k = g \).

**Remark 5.** In cases where one's primary objective is either to obtain a certificate of positive semi-definiteness or a direction of nonpositive curvature for \( A \), one can draw \( b \) from a suitably chosen random distribution, e.g., uniform distribution on the unit sphere. In this case, \( g \) satisfies the assumption of Theorem 2 with probability one.

**Top right \( (k - 1) \times (k - 1) \) block of \( R_k \)**

Theorem 1 provides a characterization for the positive-definiteness of \( T_k \) in terms of the NPC condition (9). Recall that, by Sylvester's criterion, \( T_k \succ 0 \) is a necessary and sufficient condition for the determinant of all trailing principal minors of \( T_k \) to be positive. In this light, and as a corollary of Theorem 1, the NPC condition (9) provides a characterization for the sign of such determinants. More specifically, let the determinant of the trailing principal minors of \( T_k \) be defined as

\[
p_{(k,l)} \triangleq \det \begin{bmatrix} \alpha_{k-l+1} & \beta_{k-l+2} \\ \beta_{k-l+2} & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \\ \beta_k & & & \alpha_k \end{bmatrix}, \quad 1 \leq l \leq k \leq g,
\]

where \( g \) is the grade of \( b \) with respect to \( A \). Theorem 1 implies that as long as the NPC condition (9) has not been detected after \( k \) iterations of MINRES, we have \( p_{(k,l)} > 0 \), \( l = 1, \ldots, k \).

Recall the upper-triangular matrix \( R_k \) in (6a). Clearly, by (5), we trivially get that the determinant of the trailing principal minors of \( R_k \), \( 1 \leq k \leq g \), is also positive. It turns out that we can also make a similar statement about the top right \( (k - 1) \times (k - 1) \) block of \( R_k \), namely

\[
S_k = \begin{bmatrix}
\delta^{(2)}_2 & \gamma_2 & \gamma_3^{(2)} & \cdots & \gamma_{k-1}^{(2)} & \delta_k^{(2)} \\
\gamma_2 & \delta^{(2)}_3 & \gamma_4^{(2)} & \cdots & \gamma_k^{(2)} & \\
\gamma_3^{(2)} & \gamma_4^{(2)} & \delta^{(2)}_4 & \cdots & \gamma_{k-2}^{(2)} & \\
\gamma_4^{(2)} & \gamma_5^{(2)} & \gamma_6^{(2)} & \ddots & \gamma_{k-1}^{(2)} & \\
\gamma_{k-1}^{(2)} & \gamma_k^{(2)} & \gamma_{k-2}^{(2)} & \ddots & \delta_k^{(2)} & \\
\delta_k^{(2)} & & & & & \gamma_{k-1}^{(2)}
\end{bmatrix}
\]

**Theorem 3.** Let the determinant of the trailing principal minors of \( S_k \) be defined as

\[
q_{(k,l)} \triangleq \det \begin{bmatrix} \delta^{(2)}_{k-l+1} & \epsilon_{k-l+2} \\ \gamma_{k-l+1} & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \\ \gamma_{k-1}^{(2)} & & & \delta_k^{(2)} \end{bmatrix}, \quad 1 \leq l < k \leq g.
\]

where \( g \) is the grade of \( b \) with respect to \( A \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 2 \leq k \leq g \), we must have

\[
q_{(k,l)} > 0, \quad 1 \leq l < k \leq g.
\]

**Proof.** We give an outline of the proof. The detailed proof is technical and can be found in Appendix A. The proof makes use of the three-term recurrence relation for the determinant of a tridiagonal matrix (e.g., [13, §0.9.10] and [8, Theorem 2.1]), namely

\[
q_{(l,k)} = \delta^{(2)}_{k-l+1} q_{(l-1,k)} - \gamma^{(2)}_{k-l+1} \epsilon_{k-l+2} q_{(l-2,k)}, \quad l = 1, \ldots, k - 1,
\]
where we have set \( q(k,-1) = 0 \) and \( q(k,0) = 1 \). We then consider the following ansatz for \( q(k,i) \),

\[
q(k,i) = \left( \frac{p(k,i)}{\prod_{l=1}^{i} \gamma_{k-l}^{(2)}} + \sum_{l=1}^{i} \frac{(-1)^{i-l+1} \gamma_{k-l}^{(1)} p(k,i-l)}{\prod_{j=1}^{i} \gamma_{k-j}^{(2)}} \right) \prod_{l=1}^{i} \beta_{k-l+1}, \tag{13}
\]

where \( p(k,i) \) is defined as in (10), and we set \( p(k,-1) = 0 \) and \( p(k,0) = 1 \). The proof follows by showing that (13) is indeed a correct solution to (12), which is done by induction. The last part of the proof involves showing that (13) is positive by establishing the sign of the individual terms in the sum. \( \square \)

Although Theorem 3 is a crucial ingredient in the proof of the main results of Section 3.2, it can be in fact of independent interest.

### 3.2 Monotonicity properties

When applied to positive definite systems, CG enjoys several monotonicity properties, which have historically motivated its use as subproblem solver within the optimization literature. For example, the fact that, starting with \( x_0 = 0 \), CG iterates have increasing Euclidean norm while monotonically decreasing the quadratic \( \langle x, Ax \rangle / 2 - \langle x, b \rangle \) has been heavily leveraged within the trust-region framework, e.g., CG-Steifhaug method within trust-region framework [4, 23] with \( A \) and \(-b\) being the Hessian and the gradient of the objective function, respectively. For the special case where \( A > 0 \), [9] provides such monotonicity properties for MINRES. This is done indirectly by analyzing CR and leveraging the fact that, when \( A > 0 \), MINRES and CR are in fact equivalent algorithms. In this section, we extend those results to the case where \( A \) is any symmetric and possibly indefinite and/or singular matrix. By direct analysis of the MINRES algorithm, we show that, as long as nonpositive curvature has not been detected, MINRES satisfies very similar monotonicity properties, which can be useful within various optimization frameworks. The results of this section depend on several technical lemmas, which are given in Appendix A.

Theorem 4 sheds light on the sign and monotonicity of various relevant quantities of interest. For example, from the construction of CG, when \( A > 0 \), we always have that the quadratic \( \langle x, b \rangle - \langle x, Ax \rangle / 2 \) remains positive. Theorem 4 shows that, as long as the NPC condition (9) has not been detected within MINRES, we can expect to see a similar but meaningfully different (Remark 6) quadratic to remain positive.

**Theorem 4.** Let \( g \) be the grade of \( b \) with respect to \( A \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), we have

\[
\begin{align*}
x_k^i b - x_k^i Ax_k &> 0, \quad (14a) \\
x_k^i r_k &> x_k^{i-1} r_k \geq 0, \quad (14b) \\
x_k^i r_{k-1} &> x_k^i r_k > 0, \quad (14c)
\end{align*}
\]

and the equality in (14b) holds only at \( k = 1 \).

**Proof.** We prove (14a) and (14b) by induction. For \( k = 1 \), we have

\[
x_k^1 r_1 = (x_0 + \tau_1 d_1)^T r_1 = x_0^i r_1 + \tau_1 d_1^T r_1 > x_0^i r_1 = 0,
\]

where the inequality follows from Lemma 6. Now suppose (14a) and (14b) holds for some \( k - 1 \) with \( k > 1 \). Using the fact that \( x_{k-1} \in K_{k-1}(A, b) \perp v_{k+1} \) as well as Lemma 6, we get

\[
x_k^i r_k = (x_{k-1} + \tau_k d_k)^T r_k = x_{k-1}^i r_k + \tau_k d_k^T r_k > x_{k-1}^i r_k = x_{k-1}^i (s_{k-1}^2 r_{k-1} - \phi_k c_k v_{k+1}) = s_{k-1}^2 x_{k-1}^i r_{k-1} > 0,
\]

where the last strict inequality follows from the inductive hypothesis and the fact that for any \( 1 \leq k < g \) we must have \( \beta_{k+1} \neq 0 \), which in turn implies \( s_k \neq 0 \). This gives us both (14a) and (14b).

Finally, by (16b),

\[
x_k^i r_k = x_k^i (s_{k}^2 r_{k-1} - \phi_k c_k v_{k+1}) = s_{k}^2 x_k^i r_{k-1} < x_k^i r_{k-1},
\]

which proves (14c). \( \square \)
Remark 6. Suppose \( A > 0 \). For the iterates of CG, we have \( \langle x_k, b \rangle \geq \langle x_k, Ax_k \rangle / 2 \). However, (14a) implies that the iterates of MINRES satisfy \( \langle x_k, b \rangle \geq \langle x_k, Ax_k \rangle \) (without the factor 1/2), which is a stronger property. In the context of solving \( \min_w f(w) \), this can have significant consequences for optimization algorithms that seek a descent direction at every iteration. Indeed, suppose \( A = \nabla^2 f(w) \) and \( b = -\nabla f(w) \). From (14a), it follows that the angle between the iterates of MINRES and the gradient of \( f \) is expected to be more negative than that given by the iterates of CG. In this light, loosely speaking, MINRES can produce better directions in that the amount of descent can be greater than the equivalent directions obtained from CG.

Remark 7. The conclusions of Theorem 4 hold only for when \( k < g \). For the last iteration \( k = g \), we need to consider two separate cases.

(i) When \( b \in \text{Range}(A) \), if the NPC condition (9) has not been detected for all \( g \) iterations, since \( r_g = 0 \), we get
\[
x^T_k r_{g-1} > x^T_k r_g = x^T_{g-1} r_g = 0.
\]
(ii) When \( b \notin \text{Range}(A) \), if the NPC condition (9) has not been detected for all \( g - 1 \) iterations, it is guaranteed to be detected at the \( g \)-th iteration (Lemma 2). In this case, we have \( r_g = 0 \), which implies \( r_g = 0 \), and as a result \( x_g = x_{g-1} \) and \( r_g = r_{g-1} \). Now, it can be seen from the proof of Theorem 4 that
\[
x^T_k b - x^T_k Ax_k = x^T_k r_g = x^T_{g-1} r_g = x^T_{g-1} r_{g-1} > 0.
\]

Theorem 5 provides a certain set of monotonicity results for MINRES, which for the special case of a positive definite matrix \( A \), mimic those of CG.

Theorem 5. Let \( g \) be the grade of \( b \) with respect to \( A \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), the following monotonicity results hold.

(a) If \( Ax^* = b \) for some \( x^* \in \mathbb{R}^d \), i.e., \( b \in \text{Range}(A) \), then \( \|x^* - x_k\|_A \) decreases strictly monotonically with \( k \).

(b) If \( Ax^* = b \) for some \( x^* \in \mathbb{R}^d \), i.e., \( b \in \text{Range}(A) \), then \( \|x^* - (x_{k-1} + \omega_k d_k)\|_A \) decreases strictly monotonically over \( \omega \in (-\infty, 1] \).

(c) \( m(x_k) \triangleq \langle x_k, Ax_k \rangle / 2 - \langle b, x_k \rangle \) decreases strictly monotonically with \( k \).

(d) \( m(x_{k-1} + \omega_k d_k) \) decreases strictly monotonically over \( \omega \in (-\infty, 1] \).

(e) \( \|x_k\| \) increases strictly monotonically with \( k \).

(f) \( \|x_{k-1} + \omega_k d_k\| \) decreases strictly monotonically over \( \omega \in [0, \infty) \).

(g) \( x_k^T b \) increases strictly monotonically with \( k \).

Proof.

(a) We have
\[
\|x^* - x_k\|^2_A - \|x^* - x_{k-1}\|^2_A = (x^* - x_k)^T A (x^* - x_k) - (x^* - x_{k-1})^T A (x^* - x_{k-1})
\]
\[
= -2x^T_k b + x^T_k Ax_k + 2x^T_{k-1} b - x^T_{k-1} Ax_{k-1}
\]
\[
= -2(x_{k-1}^T + \tau_k d_k) b + (x_{k-1}^T + \tau_k d_k)^T A (x_{k-1} + \tau_k d_k)
\]
\[
+ 2x^T_{k-1} b - x^T_{k-1} Ax_{k-1}
\]
\[
= -2\tau_k d_k^T b + \tau_k d_k^T Ax_k + \tau_k d_k^T Ax_{k-1} = -\tau_k d_k^T r_k - \tau_k d_k^T r_{k-1} < 0,
\]
where the last inequality comes from Lemma 6.

12
(b) Let $\omega_1 < \omega_2 \leq 1$. We have
\[
\|x^* - (x_{k-1} + \omega_2 \tau_k d_k)\|^2_A - \|x^* - (x_{k-1} + \omega_1 \tau_k d_k)\|^2_A = -2(\omega_2 - \omega_1)\tau_k d_k^T b + 2(\omega_2 - \omega_1)\tau_k A d_k = -2(\omega_2 - \omega_1)\tau_k d_k^T b + 2(\omega_2 - \omega_1)\tau_k d_k A x_{k-1} - 2(\omega_2 - \omega_1)\tau_k^2 d_k^T A d_k = -2(\omega_2 - \omega_1)\tau_k d_k^T b + 2(\omega_2 - \omega_1)\tau_k d_k A x_{k-1} - 2(\omega_2 - \omega_1)\tau_k^2 d_k^T A d_k
\]
where the last inequality follows from Lemma 6.

(c) Similar to the proof of (a), we have
\[
m(x_k) - m(x_{k-1}) = -\frac{1}{2} x_k^T b + \frac{1}{2} x_k^T A x_k + x_{k-1}^T b - \frac{1}{2} x_{k-1}^T A x_{k-1} = -\frac{1}{2} \tau_k d_k^T b + \frac{1}{2} \tau_k d_k^T A x_{k-1} + \frac{1}{2} \tau_k d_k^T A x_{k-1} = -\frac{1}{2} \tau_k d_k^T b + \frac{1}{2} \tau_k^2 d_k^T A x_{k-1} - \frac{1}{2} \tau_k \tau_k d_k^T r_k - \frac{1}{2} \tau_k d_k^T r_{k-1} < 0,
\]
where again the last inequality follows from Lemma 6.

(d) Similar to the proof of (b), let $\omega_1 < \omega_2 \leq 1$ and we have
\[
m(x_k) - m(x_{k-1}) = -\frac{1}{2} x_k^T b + \frac{1}{2} x_k^T A x_k + x_{k-1}^T b - \frac{1}{2} x_{k-1}^T A x_{k-1} = -\frac{1}{2} \tau_k d_k^T b + \frac{1}{2} \tau_k d_k^T A x_{k-1} + \frac{1}{2} \tau_k d_k^T A x_{k-1} = -\frac{1}{2} \tau_k d_k^T b + \frac{1}{2} \tau_k^2 d_k^T A x_{k-1} - \frac{1}{2} \tau_k \tau_k d_k^T r_k - \frac{1}{2} \tau_k d_k^T r_{k-1} < 0,
\]
where the last inequality comes from Lemma 6.

(e) we have
\[
\|x_k\|^2 - \|x_{k-1}\|^2 = (x_k - \tau_k d_k)^T (x_k - \tau_k d_k) - \|x_{k-1}\|^2 = 2\tau_k d_k^T x_{k-1} + \tau_k^2 d_k^T d_k = \tau_k d_k^T x_{k-1} + \tau_k^2 d_k^T d_k > 0,
\]
where the last inequality comes from Lemma 8.

(f) Let $\omega_1 < \omega_2$. We have
\[
\|x_{k-1} + \omega_2 \tau_k d_k\|^2 - \|x_{k-1} + \omega_1 \tau_k d_k\|^2 = 2(\omega_2 - \omega_1)\tau_k d_k^T x_{k-1} + (\omega_2^2 - \omega_1^2)\tau_k^2 \|d_k\|^2 > 0,
\]
where the last inequality follows from Lemma 8 and noting that $\omega_1 + \omega_2 > 0$.

(g) By Lemma 9, we simply get the result as
\[
x_k^T b - x_{k-1}^T b = \tau_k d_k^T b > 0.
\]

\[\square\]

**Remark 8.** The conclusions of Theorem 5 hold only when $k < g$. For the last iteration $k = g$, we again need to consider two separate cases.

(i) When $b \in \text{Range}(A)$, we always have $\gamma_g^{(2)} \neq 0$ (see Remark 9). In this case, if the NPC condition (9) has not been detected for all $g$ iterations, the conclusions of Theorem 5 continue to hold for $k = g$.

(ii) When $b \notin \text{Range}(A)$, as discussed in Remark 7, we always have $\gamma_g^{(2)} = 0$, $\gamma_g = 0$, and $x_g = x_{g-1}$. Also, if the NPC condition (9) has not been detected for all $g - 1$ iterations, it
is guaranteed to be detected at the $g^{th}$ iteration. This implies that at the very last iteration, we have
\[ m(x_g) = m(x_{g-1}), \quad \|x_g\| = \|x_{g-1}\|, \quad \text{and} \quad \langle x_g, b \rangle = \langle x_{g-1}, b \rangle. \]

4 Numerical experiments

We now give several numerical experiments to not only verify our main theoretical results (Section 4.1), but also to showcase the advantages of using the NPC direction detected as part of the MINRES iterations for optimization algorithms (Section 4.2).

4.1 NPC detection and monotonicity properties

In this section, we numerically verify the results from Theorems 1, 4 and 5 To do this, we consider $d = 20$ and generate symmetric matrices $A$, $B$ and $C$ as three random realizations of the Gaussian orthogonal ensemble. We then manually change the top 19 eigenvalues to be logarithmically spaced points in the interval $[1, 10^7]$. The last eigenvalues of $A$ and $B$ are set to 0 and $-1$, respectively, while the last two eigenvalues of $C$ are chosen to be $-1$ and $-10$. As a result, the first 18 positive eigenvalues of $C$ are the same as those of $A$ and $B$. We then consider solving the least-squared problem using Algorithm 1 with $b = 1$, i.e., the vector of all ones, and the underlying matrices $A$, $B$ and $C$. Figure 1 depicts several quantities of interest across the iterations of MINRES on these three problem instances.

In Figure 1, small special marks, i.e., “x”, “+”, and “•”, represent MINRES iterates, which are then connected to one another in sequence using dashed lines. The special marks corresponding to those iterations where the NPC condition (9) is detected are enlarged to distinguish them from other iterates. Let us consider all the iterates before the NPC condition (9) is detected are enlarged to distinguish them from other iterates. For all these iterations, we see that the smallest eigenvalue of $T_k$ remains strictly positive, i.e., $T_k \succ 0$, which verifies Theorem 1. Throughout these iterations, the quantity $\langle x_k, r_k \rangle$ remains positive, which validates the result of Theorem 4. Similarly, for all these iterates, as predicted by Theorem 5, the quadratic $m(x_k) \triangleq \langle x_k, Ax_k \rangle / 2 - \langle b, x_k \rangle$ is monotonically decreasing while the quantities $\|x_k\|$ and $\langle x_k, b \rangle$ are monotonically increasing. In sharp contrast, as soon as the NPC condition (9) is detected for the first time, the above monotonicity properties are no longer guaranteed and can be violated as of that iteration.

Note that, since the construction of the matrix $A$ ensures that $A \succeq 0$ and $b \notin \text{Range}(A)$, the residual of the corresponding system will not vanish, and as anticipated by Lemma 2, the NPC condition (9) is detected at the very last iteration.

4.2 NPC direction and optimization algorithms

We now move onto to present preliminary experiments to showcase advantages of using a NPC direction provided by MINRES for optimization algorithms. We do this by consider an unconstrained minimization problem involving a twice continuously differentiable function $f : \mathbb{R}^d \to \mathbb{R}$. We focus on our prior work [15, 20], henceforth referred to as $\text{Newton-MR-grad}$, as a variant of inexact Newton Method in which the least-squares subproblems are approximately solved using MINRES. By construction, $\text{Newton-MR-grad}$ solves $\min_w \|\nabla f(w)\|^2$ as a proxy for solving $\min_w f(w)$, and hence can be applied for unconstrained optimization of a class of non-convex problems known as invex [16]. However, beyond invex problems, $\text{Newton-MR-grad}$ does not provide any guarantees on the quality of the solutions and, therefore, it may terminate near a saddle point or even a local maximum. This can be remedied by employing a NPC direction arising as part of the MINRES iterations.

For this, we consider a new variant, referred to as $\text{Newton-MR}$, which differs from $\text{Newton-MR-grad}$ by two simple modifications. First, unlike $\text{Newton-MR-grad}$, the iterations of MINRES for $\text{Newton-MR}$ are terminated as soon as a NPC condition is detected and the corresponding NPC direction is return to be used for line-search purposes. Second, the Armijo-type line search is performed to obtain a step-size to reduce $f(w)$, as opposed to $\|\nabla f(w)\|^2$ for $\text{Newton-MR-grad}$. For both methods, the initial trial step-size for line-search is set to one. As a consequence of this construction, starting from the same initial point, $w_0$, both algorithms take identical steps until either a NPC direction is detected within MINRES or the step-sizes returned as part of the corresponding line-search procedures are different.
Figure 1: Several relevant quantities, namely \( \lambda_{\text{min}}(T_k), \langle x_k, r_k \rangle, m(x_k) \triangleq \langle x_k, Ax_k \rangle / 2 - \langle b, x_k \rangle, \| x_k \|, \langle x_k, b \rangle \), and \( \| r_k \| / \| b \| \), across iterations of MINRES using \( d = 20, b = 1 \), and with matrices \( A, B \) and \( C \) as constructed in Section 4.1. In all the plots, the x-axis represents the iteration counter and large special marks on each plot highlight the iterations where the NPC condition (9) is detected.

Following [28], we consider a binary classification problem using a (regularized) nonlinear least-square objective of the form

\[
    f(w) = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{1}{1 + e^{-\langle a_i, w \rangle}} - b_i \right)^2 + \psi(w),
\]

where \( \psi(w) \) is some regularization function, and the dataset \( \{a_i, b_i\}_{i=1}^{n} \) consists of feature vectors \( a_i \in \mathbb{R}^d, i = 1, \ldots, n \) and the corresponding labels \( b_i \in \{0, 1\}, i = 1, \ldots, n \). We consider three different regularization strategies, namely, a typical convex \( \ell_2 \) regularization \( \psi(w) = 0.5\|w\|^2 \), a nonconvex regularization \( \psi(w) = 0.01 \sum_{i=1}^{d} w_i^2 / (1 + w_i^2) \), and also the case where there is no regularization, \( \psi(w) = 0 \). We have used CIFAR10 dataset [14], which contains 60,000 color images of size 32 \( \times \) 32 in 10 classes. For our binary classification setting, we have relabeled the odd and even classes, respectively, as 0 and 1.

We terminate the optimization algorithms once the Euclidean norm of the gradient of \( f \) reaches below \( 10^{-10} \). The MINRES iterations are terminated if a relative residual tolerance of 0.01 is reached \( (\text{Newton-MR and Newton-MR-grad}) \) or if a NPC direction is detected \( (\text{Newton-MR}) \). To measure performance, we use the same metric as that considered in [20]. Specifically, we consider total number of oracle calls of the function, gradient and Hessian-vector product as a complexity measure. In this light, respectively, total number of oracle calls for every iteration of \( \text{Newton-MR-grad} \) and \( \text{Newton-MR} \) will be \( 2N_s + 2N_l + 2 \) and \( 2N_s + N_l + 2 \), where \( N_s \) and \( N_l \) denote the total number of iterations for MINRES and the line search.

Figure 2 shows the performance of \( \text{Newton-MR-grad} \) and \( \text{Newton-MR} \) across three regularization functions. In the plots corresponding to \( \text{Newton-MR} \), the special marks, denoted by “*”, represent iterations where MINRES detects a NPC direction, which is then used as an update direction within the line-search procedure for \( \text{Newton-MR} \). When the regularization is convex, both methods perform similarly. Despite the fact that this problem is not invex, the presence of convex regularization provides a favorable optimization landscape for \( \text{Newton-MR-grad} \), and as a result, both methods are able to find a reasonable solution with a comparative amount of work. However, beyond the convex regularization, the benefits of using NPC direction become quite clear. Indeed, the nonconvex regularization and removing regulariza-
Figure 2: The performance of Newton-MR v.s. Newton-MR-grad on the (regularized) non-linear least squares objective (15) using three different regularization strategies. The x-axis represents the total number of oracle calls. In the plots corresponding to Newton-MR, the special marks, denoted by “⋆”, represent iterations where MINRES detects a NPC direction, which is then used as an update direction within the line-search procedure.

5 Conclusions

For solving linear least-squares problems involving a real symmetric but potentially indefinite and/or singular matrix $A$, we considered the celebrated minimal residual (MINRES) method of Paige and Saunders [19]. We showed that MINRES comes equipped with an inherent ability to detect directions of nonpositive curvature. Such a direction can be detected by monitoring a certain readily available condition within the MINRES iterations (NPC Condition (9)). We showed that whenever such a condition holds, the residual of the previous iteration is one such direction. As a consequence, MINRES has a built-in mechanism to provide a certificate for the positive semi-definiteness (or lack thereof) of $A$. We then established several monotonicity properties, that mimic those of CG but are applicable for any real symmetric matrix. We also numerically verified our main results and showcased the advantages of using the NPC directions arising as part of MINRES iterations for optimization algorithms. As anticipated in [6], it is hoped that these properties will allow MINRES to be considered as a potentially superior alternative to CG for all Newton-type nonconvex optimization algorithms that employ CG as their subproblem solver.

A Technical Lemmas

To establish the main results of this paper, we need a few technical lemmas, which are all gathered here.
The following Lemmas 3 to 5 are used in the proof of Theorems 3 and 4.

**Lemma 3.** Let $g$ be the grade of $b$ with respect to $A$ as in Definition 2. As long as the NPC condition (9) has not been detected for $1 \leq k \leq g$, we have

\[
\begin{align*}
\alpha_k &> 0, \quad \beta_k > 0, \quad (16a) \\
1 > s_k &\geq 0, \quad 1 \geq |c_i| > 0, \quad (16b) \\
(-1)^{k-i}c_i\gamma_k^{(1)} &> 0, \quad (-1)^{k-i}c_i\tau_k > 0, \quad (-1)^{k-i}c_ic_k > 0, \quad 0 \leq i \leq k, \quad (16c) \\
\gamma_k^{(2)} &> 0, \quad \delta_k^{(2)} > 0, \quad \epsilon_k > 0, \quad (16d) \\
\text{Span}\{r_0, \ldots, r_{k-1}\} = \mathcal{K}_k(A, b). \quad (16e)
\end{align*}
\]

**Proof.** We first note that if the NPC condition (9) does not hold for any $k \leq g$, then we must have $c_{k-1} \neq 0$, $\phi_{k-1} \neq 0$, $\gamma_k^{(1)} \neq 0$, and consequently $\gamma_k^{(2)} \neq 0$ by (5). Also, from (7c) and Theorem 1, as long as the NPC condition (9) has not been detected for $k \leq g$, then we must have $r_{k-1}^\top A r_{k-1} > 0$ and $T_k > 0$.

By construction in Algorithm 1, we always have $\beta_k > 0$, $k \leq g$, and from $T_k > 0$ it follows that $\alpha_k > 0$, $k \leq g$. This gives (16a).

From (5) and the fact that $c_{k-1} \neq 0$, we get $0 \leq s_{k-1} < 1$ and $0 < |c_{k-1}| \leq 1$, which gives (16b).

By (5) and the construction of Algorithm 1, we know that, if $\gamma_k^{(1)} \neq 0$, then $c_i, \tau_i$ and $\gamma_k^{(1)}$ all have the same sign. Using the assumption that the NPC condition (9) does not hold, coupled with the fact that $c_0 = -1$, we get

\[
\begin{align*}
\left\{ \begin{array}{ll}
c_i > 0, \tau_i > 0, \gamma_i^{(1)} > 0, & \text{if } i \text{ is odd,} \\
c_i < 0, \tau_i < 0, \gamma_i^{(1)} < 0, & \text{if } i \text{ is even,}
\end{array} \right.
\end{align*}
\]

which gives us (16c). Again, from Algorithm 1 and (16c), we have that

\[
\gamma_k^{(2)} = \sqrt{(\gamma_k^{(1)})^2 + \beta_k^{2+1}} > 0, \quad k \geq 1,
\]

\[
\delta_k^{(2)} = -c_{k-2}c_{k-1}\beta_k + s_{k-1}\alpha_k > 0, \quad k \geq 2,
\]

\[
\epsilon_k = s_{k-2}\beta_k > 0, \quad k \geq 3,
\]

which gives (16d).

To prove (16e), we need to consider (8). If $\phi_{k-1} \neq 0$ and $c_k \neq 0$, it follows that $v_k \in \text{Span}\{r_{k-1}, r_{k-2}\}$, which in turn implies

\[
\text{Span}\{r_0, \ldots, r_{k-1}\} = \text{Span}\{v_1, \ldots, v_k\} = \mathcal{K}_k(A, b).
\]

\[\square\]

**Remark 9.** Since we always have $\beta_{g+1} = 0$, from the construction of Algorithm 1, it follows that $\gamma_g^{(2)} \neq 0$ is equivalent to having $r_g = 0$, i.e., $b \in \text{Range}(A)$. In this light, in what follows, the condition $\gamma_g^{(2)} \neq 0$ can be thought of as implying $b \in \text{Range}(A)$.

**Lemma 4.** Let $g$ be the grade of $b$ with respect to $A$ as in Definition 2. As long as the NPC condition (9) has not been detected for $1 \leq k < g$, we have

\[
(-1)^i\tau_i v_k^\top r_{k-i} > 0, \quad 0 \leq i < k, \quad 0 \leq j \leq i + 1.
\]

Furthermore, if $\gamma_g^{(2)} \neq 0$ and the NPC condition (9) has not been detected for all $g$ iterations, the conclusion continues to hold for $k = g$ and $1 \leq j \leq i + 1$. 

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17
Proof. Since $0 \leq i < k < g$, we have $\phi_{k-i-1} > 0$, which from $\phi_{k-i-1} = s_{k-i-1} s_{k-i-2} \ldots s_1 \neq 0$ and (16b) implies $0 < s_1 < 1$ for $1 \leq \ell \leq k-i-1$. Also from (16c), we have $\text{Span}(r_0, \ldots, r_{i-1}) = K_i(A, b) = \text{Span}(v_1, \ldots, v_i)$.

First, consider the case where $j = i+1 < k$. From Algorithm 1 and (16c), we have

$(-1)^j \tau_k v_{k-1}^1 r_{k-i-1} = (-1)^j \tau_k v_{k-1}^1 (s_{k-i-2} r_{k-i-2} - \phi_{k-i-1} c_{k-i-1} v_{k-i-1}) = (-1)^{i+1} \tau_k c_{k-i-1} \phi_{k-i-1} > 0.$

Now, suppose $j < i + 1 < k$. Again, from Algorithm 1 and (16c), it follows that

$$(-1)^j \tau_k v_{k-i}^j r_{k-j} = (-1)^j \tau_k v_{k-i}^j (s_{k-j} r_{k-j-1} - \phi_{k-j} c_{k-j} v_{k-j+1}) = (-1)^j \tau_k s_{k-j}^2 v_{k-j}^1 r_{k-j-1}$$

$$= (-1)^j \tau_k s_{k-j}^2 s_{k-j-1} \ldots s_{k-i}^2 v_{k-i}^1 r_{k-i-1}$$

$$= (-1)^{i+1} \tau_k c_{k-i-1} \phi_{k-i-1} \prod_{\ell=j}^{i} s_{k-\ell}^2 > 0.$$

Now, let’s suppose $j = i + 1 = k$. Similarly to above, we have

$$(-1)^{k-1} \tau_k v_{k-1}^1 r_0 = (-1)^{k-1} \tau_k \|b\| = (-1)^{k+1} \tau_k \|b\| = (-1)^k c_0 \tau_k \|b\| > 0,$$

where we have again used (16c) and the fact that $c_0 = -1$. Similarly, for $j < i + 1 = k$, we have

$$(-1)^{k-1} \tau_k v_{j}^1 r_{k-j} = (-1)^{k-1} \tau_k s_{k-j}^2 s_{k-j-1} \ldots s_1^2 v_{1}^1 r_0 = (-1)^{k-1} \tau_k s_{k-j}^2 s_{k-j-1} \ldots s_1^2 \|b\| > 0.$$

\[\square\]

**Lemma 5.** Let $g$ be the grade of $b$ with respect to $A$ as in Definition 2. We have

$$d_k = \sum_{l=0}^{k-1} \frac{(-1)^l q(k, l)}{\gamma_{k-1}^{(2)}} v_{k-l}, \quad 1 \leq k < g,$$

where $q(k, l)$ is defined in (11) and $q(k, 0) = 1$. Furthermore, if $\gamma_g^{(2)} \neq 0$, the conclusion continues to hold for $k = g$.

Proof. The proof follows by expanding the definition of $d_k$ from the construction of Algorithm 1 as well
Continuing to expand in this way, we obtain
\[
\mathbf{d}_k = \frac{1}{\gamma_k^{(2)}} \left( \mathbf{v}_k - \delta_k^{(2)} \mathbf{d}_{k-1} - \epsilon_k \mathbf{d}_{k-2} \right)
\]
\[
= \frac{1}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{\delta_k^{(2)}}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \left( \mathbf{v}_{k-1} - \delta_{k-1}^{(2)} \mathbf{d}_{k-2} - \epsilon_{k-1} \mathbf{d}_{k-3} \right) + \frac{\epsilon_k}{\gamma_k^{(2)}} \mathbf{d}_{k-2}
\]
\[
= \frac{1}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{\delta_k^{(2)}}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-1} - \frac{\delta_{k-1}^{(2)} - \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)}} \mathbf{d}_{k-2} + \frac{\epsilon_k}{\gamma_k^{(2)}} \mathbf{d}_{k-2}
\]
\[
= \frac{1}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{\delta_k^{(2)}}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-1} + \frac{\delta_{k-1}^{(2)} - \gamma_{k-2}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)}} \mathbf{d}_{k-2} + \frac{\epsilon_k}{\gamma_k^{(2)}} \mathbf{d}_{k-2}
\]
\[
= \frac{1}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{\delta_k^{(2)}}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-1} + \frac{\delta_{k-1}^{(2)} - \gamma_{k-2}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)}} \mathbf{d}_{k-2} - \epsilon_k \mathbf{d}_{k-2}
\]
\[
\delta_{k-2}^{(2)} \left( \delta_k^{(2)} - \gamma_{k-1}^{(2)} \epsilon_k \right) - \delta_{k-1}^{(2)} \epsilon_k \mathbf{d}_{k-3} = - \epsilon_k \mathbf{d}_{k-4}
\]
\[
= \frac{q(k,0)}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{q(k,1)}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-1} + \frac{q(k,2)}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-2} - \frac{q(k,2) \eta_{k-2}^{(2)} \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{d}_{k-3} - \frac{q(k,3) \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{d}_{k-4} \]
\]
Continuing to expand in this way, we obtain
\[
\mathbf{d}_k = \frac{q(k,0)}{\gamma_k^{(2)}} \mathbf{v}_k - \frac{q(k,1)}{\gamma_k^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-1} + \frac{q(k,2)}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{v}_{k-2} - \frac{q(k,3) \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{d}_{k-3} - \ldots
\]
\[
+ \frac{q(k,2) \eta_{k-2}^{(2)} \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{d}_{k-3} - \frac{q(k,3) \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)} \epsilon_k}{\gamma_k^{(2)} \gamma_{k-2}^{(2)} \gamma_{k-1}^{(2)}} \mathbf{d}_{k-4} \]
\]
\[
\vdots
\]
\[
= \sum_{i=0}^{k-1} \frac{(-1)^i q(k,i)}{\gamma_k^{(2)} \gamma_{k-1}^{(2)} \gamma_{k-2}^{(2)} \cdots \gamma_{k-i}^{(2)}} \mathbf{d}_{k-i-1}
\]
\[
= \sum_{i=0}^{k-1} \frac{(-1)^i q(k,i)}{\gamma_k^{(2)} \gamma_{k-1}^{(2)} \gamma_{k-2}^{(2)} \cdots \gamma_{k-i}^{(2)}} \mathbf{v}_{k-i-1}
\]
\[
\square
\]

**Proof of Theorem 3.** Recall the three-term recurrence relation (12) and the ansatz (13). We proceed to prove (13) by induction. By Algorithm 1, it is easy to verify that \(q(k,1)\) satisfies (13). Indeed, we have
\[
q(k,1) = \delta_k^{(2)} = c_{k-1} \delta_k^{(1)} + s_{k-1} \alpha_k = -c_{k-1} c_{k-2} \beta_k + s_{k-1} \alpha_k
\]
\[
= \gamma_k^{-1} \gamma_{k-1} \beta_k + \frac{\beta_k}{\gamma_{k-1}^{(2)}} \alpha_k = \frac{p(k,1)}{\gamma_{k-1}^{(2)}} \gamma_{k-1} - \frac{c_{k-2} \gamma_{k-1}^{(2)}}{\gamma_k^{(2)}} \beta_k
\]

By constructions in Algorithm 1 as well as (5), we have
\[
\delta_k^{(2)} = \left( c_{k-1} \delta_k^{(1)} + s_{k-1} \alpha_k \right) c_{k-2} \delta_k^{(1)} + s_{k-2} \alpha_{k-1}
\]
\[
= \left( -c_{k-1} c_{k-2} \beta_k + s_{k-1} \alpha_k \right) \left( -c_{k-2} c_{k-3} \beta_k + s_{k-2} \alpha_{k-1} \right)
\]
\[
= \left( \frac{-c_{k-2} \gamma_{k-1}^{(2)} + \alpha_k}{\gamma_k^{(2)}} \right) \left( \frac{-c_{k-3} \gamma_{k-2}^{(2)} + \alpha_k}{\gamma_k^{(2)}} \right) \beta_k \beta_{k-1}
\]
Putting this all together, it follows that

\[
q(k,2) = \delta_k^{(2)} \beta_k^{(2)} - \gamma_k^{-1} \epsilon_k
\]

\[
= \frac{\beta_{k-1} \beta_k}{\gamma_k^{-2}} \left( -c_{k-2} \gamma_k^{-1} + \alpha_k \right) \left( -c_{k-3} \gamma_k^{-1} + \alpha_k \right) - \left( \gamma_k^{-1} \right)^2 - \beta_k
\]

\[
= \frac{\beta_{k-1} \beta_k}{\gamma_k^{-2}} \left( \alpha_k - \beta_k - c_{k-3} \gamma_k^{-1} \alpha_k + \gamma_k^{-1} \left( c_{k-3} c_{k-2} \gamma_k^{-1} - c_{k-2} \alpha_k - \gamma_k^{-1} \right) \right)
\]

\[
= \frac{\beta_{k-1} \beta_k}{\gamma_k^{-2}} \left( \alpha_k - \beta_k - c_{k-3} \gamma_k^{-1} \alpha_k + c_{k-3} \gamma_k^{-1} \gamma_k^{-1} \right)
\]

where the last equality follows since

\[
\gamma_k^{-1} \left( c_{k-3} c_{k-2} \gamma_k^{-1} - c_{k-2} \alpha_k - \gamma_k^{-1} \right) = \gamma_k^{-1} \left( c_{k-3} c_{k-2} \gamma_k^{-1} + c_{k-3} \gamma_k^{-1} \gamma_k^{-1} \right) = c_{k-3} \gamma_k^{-1} \gamma_k^{-2}.
\]

Hence, it follows that \(q(k,2)\) also satisfies (13) since

\[
q(k,2) = \frac{\beta_{k-1} \beta_k}{\gamma_k^{-2}} \left( \alpha_k - \beta_k - c_{k-3} \gamma_k^{-1} \alpha_k + c_{k-3} \gamma_k^{-1} \gamma_k^{-1} \gamma_k^{-2} \right)
\]

\[
= \frac{\beta_{k-1} \beta_k}{\gamma_k^{-2}} \left( p(k,2) - c_{k-3} \gamma_k^{-2} p(k,1) + c_{k-3} \gamma_k^{-1} \gamma_k^{-2} p(k,0) \right)
\]

\[
= \left( \frac{p(k,2)}{\prod_{i=1}^2 \gamma_k^{-2}} + c_{k-3} \sum_{i=1}^{2} (-1)^{i-1} \gamma_k^{-1} \gamma_k^{-2} \sum_{j=1}^{2} \gamma_k^{-2} \right) \prod_{i=1}^2 \beta_i^{-1} + 1.
\]

Now, suppose (13) holds for \(q(k,i-1)\) and \(q(k,j-2)\) for any \(3 \leq l \leq k - 1\). By Algorithm 1 and (5), we have

\[
\delta_k^{(2)} q(k,i-1) = \left( \alpha_k - \beta_k - c_{k-3} \gamma_k^{-1} \alpha_k + c_{k-3} \gamma_k^{-1} \gamma_k^{-1} \gamma_k^{-2} \right)
\]

\[
\times \left( \frac{p(k,i-1)}{\prod_{i=1}^2 \gamma_k^{-2}} + c_{k-3} \sum_{i=1}^{2} (-1)^{i-1} \gamma_k^{-1} \gamma_k^{-2} \sum_{j=1}^{2} \gamma_k^{-2} \right) \prod_{i=1}^2 \beta_i^{-1} + 1
\]

\[
= \left( \alpha_k - \beta_k - c_{k-3} \gamma_k^{-1} \alpha_k + c_{k-3} \gamma_k^{-1} \gamma_k^{-1} \gamma_k^{-2} \right)
\]

\[
\times \left( \frac{p(k,i-1)}{\prod_{i=1}^2 \gamma_k^{-2}} + c_{k-3} \sum_{i=1}^{2} (-1)^{i-1} \gamma_k^{-1} \gamma_k^{-2} \sum_{j=1}^{2} \gamma_k^{-2} \right) \prod_{i=1}^2 \beta_i^{-1} + 1.
\]

and

\[
\gamma_k^{(2)} q(k,i-1) = \gamma_k^{(2)} \left( \beta_{k-1} \beta_k + c_{k-3} \gamma_k^{-1} \gamma_k^{-2} \right)
\]

\[
\times \left( \frac{p(k,i-1)}{\prod_{i=1}^2 \gamma_k^{-2}} + c_{k-3} \sum_{i=1}^{2} (-1)^{i-1} \gamma_k^{-1} \gamma_k^{-2} \sum_{j=1}^{2} \gamma_k^{-2} \right) \prod_{i=1}^2 \beta_i^{-1} + 1
\]

\[
= \left( \gamma_k^{(1)} \beta_{k-1} + c_{k-3} \gamma_k^{-1} \gamma_k^{-2} \right)
\]

\[
\times \left( \frac{p(k,i-1)}{\prod_{i=1}^2 \gamma_k^{-2}} + c_{k-3} \sum_{i=1}^{2} (-1)^{i-1} \gamma_k^{-1} \gamma_k^{-2} \sum_{j=1}^{2} \gamma_k^{-2} \right) \prod_{i=1}^2 \beta_i^{-1} + 1.
\]
We now verify that (13) is indeed the difference of (17) and (18) and hence agrees with (12). Factoring out the common term \( \prod_{i=1}^{l} \beta_{k-i+1} \), we now combine and simplify some terms in this difference.

We first note that
\[
\frac{\alpha_{k-l+1}}{\gamma_{k-l}} \frac{P(k,l-1)}{\prod_{i=1}^{l-1} \gamma_{k-i}} - \frac{\beta_{k-l}^2}{\gamma_{k-l+1} \gamma_{k-l}} \frac{P(k,l-2)}{\prod_{i=1}^{l-2} \gamma_{k-i}} = \frac{\alpha_{k-l+1} P(k,l-1) - \beta_{k-l+2}^2 P(k,l-2)}{\prod_{i=1}^{l} \gamma_{k-i}} = \frac{P(k,l)}{\prod_{i=1}^{l} \gamma_{k-i}},
\]
and
\[
-\frac{c_k - l \gamma_{k-l}^1}{\gamma_{k-l}^{(2)}} \prod_{i=1}^{l-1} \gamma_{k-i} = -\frac{c_k - l \gamma_{k-l}^1 \prod_{i=1}^{l-2} \gamma_{k-i}}{\prod_{i=1}^{l-2} \gamma_{k-i}}.
\]

We have
\[
-(\alpha_{k-l+1} - c_k - l \gamma_{k-l}^1) c_k - l \gamma_{k-l+1} - \gamma_{k-l+1}^2
\]
\[
= \gamma_{k-l+1}^2 (-c_k - l \alpha_{k-l+1} + c_k - l c_k - l \gamma_{k-l}^1) - (-c_k - l s_{k-l} \beta_{k-l+1} - c_k - l \alpha_{k-l+1})
\]
\[
= c_k - l \gamma_{k-l+1}^1 (c_k - l \gamma_{k-l}^1 + s_{k-l} \beta_{k-l+1}) = c_k - l \gamma_{k-l+1}^1 \gamma_{k-l}^2 = c_k - l \gamma_{k-l+1}^2 \gamma_{k-l}.
\]

This gives
\[
\left(\frac{\alpha_{k-l+1} - c_k - l \gamma_{k-l}^1}{\gamma_{k-l}} \right) \left(\frac{-c_k - l \gamma_{k-l}^1 \prod_{i=1}^{l-2} \gamma_{k-i}}{\gamma_{k-l+1} \gamma_{k-l} \prod_{i=1}^{l-2} \gamma_{k-i}}\right) = \frac{c_k - l \gamma_{k-l+1}^1 \prod_{i=1}^{l-2} \gamma_{k-i}}{\prod_{i=1}^{l-2} \gamma_{k-i}}.
\]

Finally, for any \( 1 \leq i \leq l - 2 \), we have
\[
\left(\frac{\alpha_{k-l+1} - c_k - l \gamma_{k-l}^1}{\gamma_{k-l}} \right) \left(\frac{c_k - l (-1)^{l-i-1} \gamma_{k-l}^1 \prod_{j=1}^{i} \gamma_{k-j}}{\prod_{j=1}^{i} \gamma_{k-j}}\right) = \frac{c_k - l \gamma_{k-l+1} \prod_{j=1}^{i} \gamma_{k-j}}{\prod_{j=1}^{i} \gamma_{k-j}}.
\]

Now, summing up (19) to (22), and putting \( \prod_{i=1}^{l} \beta_{k-i+1} \) factor back in, we obtain (13). The claim follows by noticing that from Theorem 1, (16c) and (16d), all of (19) to (22) evaluate to be positive. Furthermore, by (16a), we also have \( \prod_{i=1}^{l} \beta_{k-i+1} > 0 \). Putting this all together, we get the desired result. \( \square \)

Lemma 6 allow us to make a statement about the “angle” between the update vector \( \tau_k d_k \) and the residual vectors, which is used in the proofs of Theorems 4 and 5.

**Lemma 6.** Let \( g \) be the grade of \( b \) with respect to \( A \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), we have
\[
\tau_k d_k \beta_{k-j} > 0, \quad 0 \leq j < k.
\]

Furthermore, if \( \gamma_{g}^{(2)} \neq 0 \) and the NPC condition (9) has not been detected for all \( g \) iterations, the...
Proof. This easily follows from Lemmas 4 and 5, Theorem 3, and (16d), because

\[ \tau_k \mathbf{d}_k^{\tau} \mathbf{x}_{k-j} = \tau_k \sum_{i=0}^{k-1} \frac{(-1)^i q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \mathbf{v}_{k-i}^\top \mathbf{r}_{k-j} > 0, \]

where we also used the fact that \( \mathbf{v}_{k-i} \perp \mathbf{r}_{k-j}, \ i < j - 1. \)

The following technical lemmas (Lemmas 7 to 9) will be used in the proof of Theorem 5.

**Lemma 7.** Let \( g \) be the grade of \( \mathbf{b} \) with respect to \( \mathbf{A} \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), we have

\[ (-1)^j \tau_k \mathbf{d}_{k-j}^\tau \mathbf{v}_{k-i} > 0, \quad 0 \leq j \leq k. \]

Furthermore, if \( \gamma_g^{(2)} \neq 0 \) and the NPC condition (9) has not been detected for all \( g \) iterations, the conclusion continues to hold for \( k = g \).

**Proof.** By Lemma 5, we have

\[ \mathbf{v}_{k-i}^\top \mathbf{d}_{k-j} = \mathbf{v}_{k-i}^\top \left( \sum_{h=0}^{k-j-1} \frac{(-1)^h q(k-j,h)}{\prod_{\ell=0}^{(2)} \gamma_{k-j-h+\ell}} \mathbf{v}_{k-j-h} \right) = \frac{(-1)^{i-j} q(k-j,i-j)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}}. \]

Also, by (16c) and the definition of \( \tau_k \) in Algorithm 1, we have

\[ (-1)^{-j} \tau_k \mathbf{d}_{k-j}^\tau \mathbf{v}_{k-i} = (-1)^j \tau_k \mathbf{d}_{k-j}^\tau \mathbf{v}_{k-i} = (-1)^{-j} \tau_k \mathbf{d}_{k-j}^\tau \mathbf{v}_{k-i} = (-1)^{-j} \tau_k \mathbf{d}_{k-j}^\tau \mathbf{v}_{k-i} > 0. \]

**Lemma 8.** Let \( g \) be the grade of \( \mathbf{b} \) with respect to \( \mathbf{A} \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), we have

\[ \tau_k \mathbf{d}_k^{\tau} \mathbf{x}_{k-j} > 0, \quad 0 \leq j < k. \]

Furthermore, if \( \gamma_g^{(2)} \neq 0 \) and the NPC condition (9) has not been detected for all \( g \) iterations, the conclusion continues to hold for \( k = g \).

**Proof.** By Lemma 5 and noting that \( \mathbf{x}_k \in K_k(\mathbf{A}, \mathbf{b}) \perp \mathbf{v}_{k-i+1} \), we have

\[ \tau_k \mathbf{d}_k^{\tau} \mathbf{x}_{k-j} = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \mathbf{v}_{k-i}^\top \mathbf{x}_{k-j} = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \mathbf{v}_{k-i}^\top \mathbf{x}_{k-j} \]

\[ = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \mathbf{v}_{k-i}^\top \left( \mathbf{r}_{k-i}^{\tau} \mathbf{v}_{k-i} \right) = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \sum_{h=0}^{k-j} \tau_h \mathbf{d}_h. \]

Again from Lemma 5, we have

\[ \mathbf{v}_{k-i}^\top \mathbf{d}_h = \mathbf{v}_{k-i}^\top \left( \sum_{h=0}^{k-1} \frac{(-1)^i \tau_k q(h,i)}{\prod_{\ell=0}^{(2)} \gamma_{h-i+\ell}} \mathbf{v}_{h-i} \right) = 0, \quad h < k - i, \]

which implies

\[ \tau_k \mathbf{d}_k^{\tau} \mathbf{x}_{k-j} = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \left( \sum_{h=0}^{k-j} \tau_h \mathbf{d}_h \right) = \sum_{i=0}^{k-1} \frac{(-1)^i \tau_k q(k,i)}{\prod_{\ell=0}^{(2)} \gamma_{k-i+\ell}} \left( \tau_k \mathbf{d}_k^{\tau} \mathbf{v}_{k-i} \right) > 0, \]

where the last inequality follows from Theorem 3, (16d), and Lemma 7.
Lemma 9. Let \( g \) be the grade of \( b \) with respect to \( A \) as in Definition 2. As long as the NPC condition (9) has not been detected for \( 1 \leq k < g \), we have
\[
\tau_k d_k b > 0.
\]
Furthermore, if \( \gamma^{(2)}_g \neq 0 \) and the NPC condition (9) has not been detected for all \( g \) iterations, the conclusion continues to hold for \( k = g \).

Proof. By Lemma 5, we have
\[
\tau_k d_k b = \beta_1 \left( \sum_{i=0}^{k-1} q(k,i) \prod_{\ell=0}^{i-1} \gamma^{(2)}_{k-i+\ell} (-1)^i \tau_k v_{k-i} \right)^\top v_1
\]
\[
= \frac{q(k,k-1)}{\prod_{\ell=0}^{k-1} \gamma^{(2)}_{k+\ell}} (-1)^{k-1} \tau_k v_1^\top v_1 = \frac{\beta_1 q(k,k-1)}{\prod_{\ell=0}^{k-1} \gamma^{(2)}_{k+\ell}} (-1)^k c_0 \tau_k > 0,
\]
where the last inequality comes from (16c).

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