# MINRES-QLP: A KRYLOV SUBSPACE METHOD FOR INDEFINITE OR SINGULAR SYMMETRIC SYSTEMS* 

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#### Abstract

CG, SYMMLQ, and MINRES are Krylov subspace methods for solving symmetric systems of linear equations. When these methods are applied to an incompatible system (that is, a singular symmetric least-squares problem), CG could break down and SYMMLQ's solution could explode, while MINRES would give a least-squares solution but not necessarily the minimum-length (pseudoinverse) solution. This understanding motivates us to design a MINRES-like algorithm to compute minimum-length solutions to singular symmetric systems.

MINRES uses QR factors of the tridiagonal matrix from the Lanczos process (where $R$ is uppertridiagonal). MINRES-QLP uses a QLP decomposition (where rotations on the right reduce $R$ to lower-tridiagonal form). On ill-conditioned systems (singular or not), MINRES-QLP can give more accurate solutions than MINRES. We derive preconditioned MINRES-QLP, new stopping rules, and better estimates of the solution and residual norms, the matrix norm, and the condition number.


Key words. MINRES, Krylov subspace method, Lanczos process, conjugate-gradient method, minimum-residual method, singular least-squares problem, sparse matrix

AMS subject classifications. 15A06, 65F10, 65F20, 65F22, 65F25, 65F35, 65F50, 93E24
DOI. $x x x / x x y x x x x x x$

1. Introduction. We are concerned with iterative methods for solving a symmetric linear system $A x=b$ or the related least-squares (LS) problem

$$
\begin{equation*}
\min \|x\|_{2} \quad \text { s.t. } \quad x \in \arg \min _{x}\|A x-b\|_{2}, \tag{1.1}
\end{equation*}
$$

where $A \in \mathbb{R}^{n \times n}$ is symmetric and possibly singular, $b \in \mathbb{R}^{n}, A \neq 0$, and $b \neq 0$. Most of the results in our discussion are directly extendable to problems with complex Hermitian matrices $A$ and complex vectors $b$.

The solution of (1.1), called the minimum-length or pseudoinverse solution [18], is formally given by $x^{\dagger}=\left(A^{T} A\right)^{\dagger} A^{T} b=\left(A^{2}\right)^{\dagger} A b=\left(A^{\dagger}\right)^{2} A b$, where $A^{\dagger}$ denotes the pseudoinverse of $A$. The pseudoinverse is continuous under perturbations $E$ for which $\operatorname{rank}(A+E)=\operatorname{rank}(A)$ [49], and $x^{\dagger}$ is continuous under the same condition. Problem (1.1) is then well-posed [19].

Let $A=U \Lambda U^{T}$ be an eigenvalue decomposition of $A$, with $U$ orthogonal and $\Lambda \equiv \operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{n}\right)$. We define the condition number of $A$ to be $\kappa(A)=\frac{\max \left|\lambda_{i}\right|}{\min _{\lambda_{i} \neq 0}\left|\lambda_{i}\right|}$, and we say that $A$ is ill-conditioned if $\kappa(A) \gg 1$. Hence a singular matrix could be well-conditioned or ill-conditioned.

[^0]SYMMLQ and MINRES [39] are Krylov subspace methods for solving symmetric indefinite systems $A x=b$. SYMMLQ is reliable on compatible systems even if $A$ is ill-conditioned or singular, while on (singular) incompatible problems its iterates $x_{k}$ diverge to a multiple of a nullvector of $A$ [10, Proposition 2.15] and [10, Lemma 2.17]. MINRES seems more desirable to users because its residual norms are monotonically decreasing. On singular compatible systems, MINRES returns $x^{\dagger}$ (see Theorem 3.1). On singular incompatible systems, MINRES is reliable if terminated with a suitable stopping rule involving $\left\|A r_{k}\right\|$ (see Lemma 3.3), but the solution will not be $x^{\dagger}$.

Here we develop a new solver of this type named MINRES-QLP [10]. The aim is to deal reliably with compatible or incompatible systems and to return the unique solution of (1.1). We give theoretical reasons why MINRES-QLP improves the accuracy of MINRES on ill-conditioned systems, and illustrate with numerical examples.

Incompatible symmetric systems could arise from discretized semidefinite Neumann boundary value problems [27, section 4], and from any other singular systems involving measurement errors in $b$. Another potential application is large symmetric indefinite low-rank Toeplitz LS problems as described in [16, section 4.1].
1.1. Notation. The letters $i, j, k$ denote integer indices, $c$ and $s$ cosine and sine of some angle $\theta, e_{k}$ the $k$ th unit vector, $e$ a vector of all ones, and other lower-case letters such as $b, u$, and $x$ (possibly with integer subscripts) denote column vectors. Upper-case letters $A, T_{k}, V_{k}, \ldots$ denote matrices, and $I_{k}$ is the identity matrix of order $k$. Lower-case Greek letters denote scalars; in particular, $\varepsilon \approx 10^{-16}$ denotes the floating-point precision. If a quantity $\delta_{k}$ is modified one or more times, we denote its values by $\delta_{k}, \delta_{k}^{(2)}, \delta_{k}^{(3)}, \ldots$ The symbol $\|\cdot\|$ denotes the 2 -norm of a vector or matrix. For an incompatible system, $A x \approx b$ is shorthand for the LS problem $\min _{x}\|A x-b\|$.
1.2. Overview. In sections $2-4$ we briefly review the Lanczos process, MINRES, and QLP decomposition before introducing MINRES-QLP in section 5. We derive norm estimates in section 6 and preconditioned MINRES-QLP in section 7. Numerical experiments are described in section 8.
2. The Lanczos process. Given $A$ and $b$, the Lanczos process [30] computes vectors $v_{k}$ and tridiagonal matrices $\underline{T_{k}}$ according to $v_{0} \equiv 0, \beta_{1} v_{1}=b$, and then ${ }^{1}$

$$
p_{k}=A v_{k}, \quad \alpha_{k}=v_{k}^{T} p_{k}, \quad \beta_{k+1} v_{k+1}=p_{k}-\alpha_{k} v_{k}-\beta_{k} v_{k-1}
$$

for $k=1,2, \ldots, \ell$, where we choose $\beta_{k}>0$ to give $\left\|v_{k}\right\|=1$. In matrix form,

$$
A V_{k}=V_{k+1} \underline{T_{k}}, \quad \underline{T_{k}} \equiv\left[\begin{array}{cccc}
\alpha_{1} & \beta_{2} & &  \tag{2.1}\\
\beta_{2} & \alpha_{2} & \ddots & \\
& \ddots & \ddots & \beta_{k} \\
& & \beta_{k} & \alpha_{k} \\
& & & \beta_{k+1}
\end{array}\right] \equiv\left[\begin{array}{c}
T_{k} \\
\beta_{k+1} e_{k}^{T}
\end{array}\right], \quad V_{k} \equiv\left[\begin{array}{lll}
v_{1} & \cdots & v_{k}
\end{array}\right]
$$

In exact arithmetic, the columns of $V_{k}$ are orthonormal and the process stops with $k=\ell$ and $\beta_{\ell+1}=0$ for some $\ell \leq n$, and then $A V_{\ell}=V_{\ell} T_{\ell}$. For derivation purposes we assume that this happens, though in practice it is unlikely unless $V_{k}$ is reorthogonalized for each $k$. In any case, (2.1) holds to machine precision and the computed vectors satisfy $\left\|V_{k}\right\|_{1} \approx 1$ (even if $k \gg n$ ).

[^1]2.1. Properties of the Lanczos process. The $k$ th Krylov subspace generated by $A$ and $b$ is defined to be $\mathcal{K}_{k}(A, b)=\operatorname{span}\left\{b, A b, A^{2} b, \ldots, A^{k-1} b\right\}=\operatorname{span}\left(V_{k}\right)$. The following properties should be kept in mind:

1. If $A$ is changed to $A-\sigma I$ for some scalar shift $\sigma, T_{k}$ becomes $T_{k}-\sigma I$ and $V_{k}$ is unaltered, showing that singular systems are commonplace. Shifted problems appear in inverse iteration or Rayleigh quotient iteration.
2. $T_{k}$ has full column rank $k$ for all $k<\ell$.
3. If $A$ is indefinite, some $T_{k}$ might be singular for $k<\ell$, but then by the Sturm sequence property (see [18]), $T_{k}$ has exactly one zero eigenvalue and the strict interlacing property implies that $T_{k \pm 1}$ are nonsingular. Hence $T_{k}$ cannot be singular twice in a row (whether $A$ is singular or not).
4. $T_{\ell}$ is nonsingular if and only if $b \in \operatorname{range}(A)$. (See appendix A.)
5. MINRES. Algorithm MINRES [39] is a natural way of using the Lanczos process to solve $A x=b$ or $\min _{x}\|A x-b\|$. For $k<\ell$, if $x_{k}=V_{k} y_{k}$ for some vector $y_{k}$, the associated residual is

$$
\begin{equation*}
r_{k} \equiv b-A x_{k}=b-A V_{k} y_{k}=\beta_{1} v_{1}-V_{k+1} \underline{T_{k}} y_{k}=V_{k+1}\left(\beta_{1} e_{1}-\underline{T_{k}} y_{k}\right) . \tag{3.1}
\end{equation*}
$$

To make $r_{k}$ small, it is clear that $\beta_{1} e_{1}-\underline{T_{k}} y_{k}$ should be small. At this iteration $k$, MINRES minimizes the residual subject to $x_{k} \in \mathcal{K}_{k}(A, b)$ by choosing

$$
\begin{equation*}
y_{k}=\arg \min _{y \in \mathbb{R}^{k}}\left\|\underline{T_{k}} y-\beta_{1} e_{1}\right\| . \tag{3.2}
\end{equation*}
$$

This subproblem is processed by the expanding QR factorization: $Q_{0} \equiv 1$ and

$$
Q_{k, k+1} \equiv\left[\begin{array}{ccc}
I_{k-1} & &  \tag{3.3}\\
& c_{k} & s_{k} \\
& s_{k}-c_{k}
\end{array}\right], \quad Q_{k} \equiv Q_{k, k+1}\left[\begin{array}{ll}
Q_{k-1} & \\
& 1
\end{array}\right], \quad Q_{k}\left[\underline{T_{k}} \quad \beta_{1} e_{1}\right]=\left[\begin{array}{cc}
R_{k} & t_{k} \\
0 & \phi_{k}
\end{array}\right],
$$

where $c_{k}$ and $s_{k}$ form the Householder reflector $Q_{k, k+1}$ that annihilates $\beta_{k+1}$ in $\underline{T_{k}}$ to give upper-tridiagonal $R_{k}$, with $R_{k}$ and $t_{k}$ being unaltered in later iterations.

When $k<\ell$, the unique solution of (3.2) satisfies $R_{k} y_{k}=t_{k}$. Instead of solving for $y_{k}$, MINRES solves $R_{k}^{T} D_{k}^{T}=V_{k}^{T}$ by forward substitution, obtaining the last column $d_{k}$ of $D_{k}$ at iteration $k$. At the same time, it updates $x_{k}$ via $x_{0} \equiv 0$ and

$$
\begin{equation*}
x_{k}=V_{k} y_{k}=D_{k} R_{k} y_{k}=D_{k} t_{k}=x_{k-1}+\tau_{k} d_{k}, \quad \tau_{k} \equiv e_{k}^{T} t_{k} \tag{3.4}
\end{equation*}
$$

When $k=\ell$, we can form $T_{\ell}$ but nothing else expands. In place of (3.1) and (3.3) we have $r_{\ell}=V_{\ell}\left(\beta_{1} e_{1}-T_{\ell} y_{\ell}\right)$ and $Q_{\ell-1}\left[\begin{array}{ll}T_{\ell} & \beta_{1} e_{1}\end{array}\right]=\left[\begin{array}{ll}R_{\ell} & t_{\ell}\end{array}\right]$ and it is natural to choose $y_{\ell}$ from the subproblem

$$
\begin{equation*}
\min \left\|T_{\ell} y_{\ell}-\beta_{1} e_{1}\right\| \equiv \min \left\|R_{\ell} y_{\ell}-t_{\ell}\right\| \tag{3.5}
\end{equation*}
$$

There are two cases to consider:

1. If $T_{\ell}$ is nonsingular, $R_{\ell} y_{\ell}=t_{\ell}$ has a unique solution. Since $A V_{\ell} y_{\ell}=V_{\ell} T_{\ell} y_{\ell}=$ $b$, the problem is solved by $x_{\ell}=V_{\ell} y_{\ell}$ with residual $r_{\ell}=0$ (the system is compatible, even if $A$ is singular). Theorem 3.1 proves that $x_{\ell}=x^{\dagger}$.
2. If $T_{\ell}$ is singular, $A$ and $R_{\ell}$ are singular $\left(R_{\ell \ell}=0\right)$ and both $A x=b$ and $R_{\ell} y_{\ell}=t_{\ell}$ are incompatible. This case was not handled by MINRES in [39]. Theorem 3.2 proves that the MINRES point $x_{\ell-1}$ is a least-squares solution (but not necessarily $x^{\dagger}$ ). Theorem 5.1 proves that the MINRES-QLP point $x_{\ell}=V_{\ell} y_{\ell}^{\dagger}=x^{\dagger}$, where $y_{\ell}^{\dagger}$ is the min-length solution of (3.5).
3.1. Further details of MINRES. To describe MINRES-QLP thoroughly, we need further details of the MINRES QR factorization (3.3). For $1 \leq k<\ell$,

$$
\left[\begin{array}{c}
R_{k}  \tag{3.6}\\
0
\end{array}\right]=\left[\begin{array}{ccccc}
\gamma_{1} & \delta_{2} & \epsilon_{3} & & \\
& \gamma_{2}^{(2)} & \delta_{3}^{(2)} & \ddots & \\
& & \ddots & \ddots & \epsilon_{k} \\
& & & \ddots & \delta_{k}^{(2)} \\
& & & & \gamma_{k}^{(2)} \\
& & & & 0
\end{array}\right], \quad\left[\begin{array}{c}
t_{k} \\
\phi_{k}
\end{array}\right] \equiv\left[\begin{array}{c}
\tau_{1} \\
\tau_{2} \\
\vdots \\
\vdots \\
s_{1} c_{2} \\
\vdots \\
\tau_{k} \\
\phi_{k}
\end{array}\right]=\beta_{1}\left[\begin{array}{c}
c_{1} \\
\vdots \\
s_{1} \cdots s_{k-1} c_{k} \\
s_{1} \cdots s_{k-1} s_{k}
\end{array}\right]
$$

(where the superscripts are defined in section 1.1). With $\phi_{0} \equiv \beta_{1}>0$, the full action of $Q_{k, k+1}$ in (3.3), including its effect on later columns of $T_{j}, k<j \leq \ell$, is described by

$$
\left[\begin{array}{rr}
c_{k} & s_{k}  \tag{3.7}\\
s_{k} & -c_{k}
\end{array}\right]\left[\begin{array}{ccc|c}
\gamma_{k} & \delta_{k+1} & 0 & \phi_{k-1} \\
\beta_{k+1} & \alpha_{k+1} & \beta_{k+2} & 0
\end{array}\right]=\left[\begin{array}{ccc|c}
\gamma_{k}^{(2)} & \delta_{k+1}^{(2)} & \epsilon_{k+2} & \tau_{k} \\
0 & \gamma_{k+1} & \delta_{k+2} & \phi_{k}
\end{array}\right]
$$

where $s_{k}=\beta_{k+1} /\left\|\left[\begin{array}{ll}\gamma_{k} & \beta_{k+1}\end{array}\right]\right\|>0$, giving $\gamma_{1}, \gamma_{k}^{(2)}>0$ with $R_{j}$ nonsingular for each $j \leq k<\ell$. Thus the $d_{j}$ in (3.4) can be found from

$$
R_{k}^{T} D_{k}^{T}=V_{k}^{T}:\left\{\begin{array}{l}
d_{1}=v_{1} / \gamma_{1}, \quad d_{2}=\left(v_{2}-\delta_{2} d_{1}\right) / \gamma_{2}^{(2)},  \tag{3.8}\\
d_{j}=\left(v_{j}-\delta_{j}^{(2)} d_{j-1}-\epsilon_{j} d_{j-2}\right) / \gamma_{j}^{(2)}, \quad j=3, \ldots, k
\end{array}\right.
$$

Also, $\tau_{k}=\phi_{k-1} c_{k}$ and $\phi_{k}=\phi_{k-1} s_{k}>0$. Hence from (3.1)-(3.3),

$$
\begin{equation*}
\left\|r_{k}\right\|=\left\|\underline{T_{k}} y_{k}-\beta_{1} e_{1}\right\|=\phi_{k} \quad \Rightarrow \quad\left\|r_{k}\right\|=\left\|r_{k-1}\right\| s_{k} \tag{3.9}
\end{equation*}
$$

which is nonincreasing and tending to zero if $A x=b$ is compatible.
Remark 3.1. If $k<\ell$ and $T_{k}$ is singular, we have $\gamma_{k}=0$, $s_{k}=1$, and $\left\|r_{k}\right\|=$ $\left\|r_{k-1}\right\|$ (not a strict decrease), but this cannot happen twice in a row (cf. section 2.1).

REMARK 3.2. If $T_{\ell}$ is singular, MINRES sets the last element of $y_{\ell}$ to be zero. The final point and residual stay as $x_{\ell-1}$ and $r_{\ell-1}$ with $\left\|r_{\ell-1}\right\|=\phi_{\ell-1}=\beta_{1} s_{1} \cdots s_{\ell-1}>0$.
3.2. Compatible systems. The following theorem assures us that MINRES is a useful solver for compatible linear systems even if $A$ is singular.

Theorem 3.1 ([10, Theorem 2.25]). If $b \in \operatorname{range}(A)$, the final MINRES point $x_{\ell}$ is the minimum-length solution of $A x=b$ (and $r_{\ell}=b-A x_{\ell}=0$ ).

Proof. If $b \in \operatorname{range}(A)$, the Lanczos process gives $A V_{\ell}=V_{\ell} T_{\ell}$ with nonsingular $T_{\ell}$, and MINRES terminates with $A x_{\ell}=b$ and $x_{\ell}=V_{\ell} y_{\ell}=A q$, where $q=V_{\ell} T_{\ell}^{-1} y_{\ell}$. If some other point $\widehat{x}$ satisfies $A \widehat{x}=b$, let $p=\widehat{x}-x_{\ell}$. We have $A p=0$ and $x_{\ell}^{T} p=q^{T} A p=0$. Hence $\|\widehat{x}\|^{2}=\left\|x_{\ell}+p\right\|^{2}=\left\|x_{\ell}\right\|^{2}+2 x_{\ell}^{T} p+\|p\|^{2} \geq\left\|x_{\ell}\right\|^{2}$.
3.3. Incompatible systems. For a singular LS problem $A x \approx b$, the optimal residual vector $\widehat{r}$ is unique, but infinitely many solutions $x$ give that residual. In the following example, MINRES finds a least-squares solution (with optimal residual) but not the minimum-length solution.

Example 3.1. Let $A=\operatorname{diag}(1,1,0)$ and $b=e$. The minimum-length solution to $A x \approx b$ is $x^{\dagger}=\left[\begin{array}{lll}1 & 1 & 0\end{array}\right]^{T}$ with residual $\widehat{r}=b-A x^{\dagger}=e_{3}$ and $A \widehat{r}=0$. MINRES returns the solution $x^{\sharp}=e\left(\right.$ with residual $r^{\sharp}=b-A x^{\sharp}=e_{3}=\widehat{r}$ and $\left.A r^{\sharp}=0\right)$.

Theorem 3.2 ([10, Theorem 2.27]). If $b \notin$ range $(A)$, then $\left\|A r_{\ell-1}\right\|=0$ and the MINRES $x_{\ell-1}$ is an $L S$ solution (but not necessarily $x^{\dagger}$ ).

Proof. Since $b \notin \operatorname{range}(A), T_{\ell}$ is singular and $R_{\ell \ell}=\gamma_{\ell}=0$. By Lemma 3.3 below, $A\left(A x_{\ell-1}-b\right)=-A r_{\ell-1}=-\left\|r_{\ell-1}\right\| \gamma_{\ell} v_{\ell}=0$. Thus $x_{\ell-1}$ is an LS solution.
3.4. Norm estimates in MINRES. For incompatible systems, $r_{k}$ (3.1) will never be zero. However, all LS solutions satisfy $A^{2} x=A b$, so that $A r=0$. We therefore need a new stopping condition based on the size of $\left\|A r_{k}\right\|$. In applications requiring nullvectors, $\left\|A x_{k}\right\|$ is also useful. We present efficient recurrence relations for $\left\|A r_{k}\right\|$ and $\left\|A x_{k}\right\|$ in the following Lemma, which was not considered in the framework of MINRES when it was originally designed for nonsingular systems [39].

Lemma $3.3\left(A r_{k},\left\|A r_{k}\right\|,\left\|A x_{k}\right\|\right.$ for MINRES). If $k<\ell$,

$$
\begin{array}{rlr}
A r_{k} & =\left\|r_{k}\right\|\left(\gamma_{k+1} v_{k+1}+\delta_{k+2} v_{k+2}\right) \quad\left(\text { where } \delta_{k+2} v_{k+2}=0 \text { if } k=\ell-1\right), \\
\psi_{k}^{2} & \equiv\left\|A r_{k}\right\|^{2}=\left\|r_{k}\right\|^{2}\left(\left[\gamma_{k+1}\right]^{2}+\left[\delta_{k+2}\right]^{2}\right) \quad\left(\text { where } \delta_{k+2}=0 \text { if } k=\ell-1\right), \\
\omega_{k}^{2} & \equiv\left\|A x_{k}\right\|^{2}=\omega_{k-1}^{2}+\tau_{k}^{2}, \quad \omega_{0} \equiv 0
\end{array}
$$

Proof. For $k<\ell, R_{k}$ is nonsingular. From (3.1)-(3.4) with $R_{k} y_{k}=t_{k}$ we have

$$
\begin{align*}
r_{k} & =V_{k+1} Q_{k}^{T}\left(\left[\begin{array}{c}
t_{k} \\
\phi_{k}
\end{array}\right]-\left[\begin{array}{c}
R_{k} \\
0
\end{array}\right] y_{k}\right)=\phi_{k} V_{k+1} Q_{k}^{T} e_{k+1},  \tag{3.10}\\
A r_{k} & =\phi_{k} V_{k+2} \underline{T_{k+1}} Q_{k}^{T} e_{k+1}, \\
Q_{k} \underline{T_{k+1}}{ }^{T} & =Q_{k}\left[\begin{array}{ll}
T_{k+1} & \beta_{k+2} e_{k+1}
\end{array}\right]=Q_{k}\left[\begin{array}{ccc}
T_{k} & \beta_{k+1} e_{k} & 0 \\
\beta_{k+1} e_{k}^{T} & \alpha_{k+1} & \beta_{k+2}
\end{array}\right], \\
e_{k+1}^{T} Q_{k} \underline{T_{k+1}} & =\left[\begin{array}{lll}
0 & \gamma_{k+1} & \delta_{k+2}
\end{array}\right],
\end{align*}
$$

see (3.7), where $A V_{k+1}=V_{k+1} T_{k+1}$ and we take $\delta_{k+2}=0$ if $k=\ell-1$, so

$$
\begin{aligned}
A r_{k} & =\phi_{k} V_{k+2}\left[\begin{array}{lll}
0 & \gamma_{k+1} & \delta_{k+2}
\end{array}\right]^{T}=\phi_{k}\left(\gamma_{k+1} v_{k+1}+\delta_{k+2} v_{k+2}\right) \\
\psi_{k}^{2} & \equiv\left\|A r_{k}\right\|^{2}=\left\|r_{k}\right\|^{2}\left(\left[\gamma_{k+1}\right]^{2}+\left[\delta_{k+2}\right]^{2}\right)
\end{aligned}
$$

For the recurrence relations of $A x_{k}$ and its norm, we have

$$
\begin{aligned}
A x_{k} & =A V_{k} y_{k}=V_{k+1} \underline{T_{k}} y_{k}=V_{k+1} Q_{k}^{T}\left[\begin{array}{c}
R_{k} \\
0
\end{array}\right] y_{k}=V_{k+1} Q_{k}^{T}\left[\begin{array}{c}
t_{k} \\
0
\end{array}\right] \\
\omega_{k}^{2} & \equiv\left\|A x_{k}\right\|^{2}=\left\|t_{k}\right\|^{2}=\left\|t_{k-1}\right\|^{2}+\tau_{k}^{2}=\omega_{k-1}^{2}+\tau_{k}^{2}
\end{aligned}
$$

Note that even using finite precision the expression for $\psi_{k}^{2}$ is extremely accurate for the versions of the Lanczos algorithm given in section 2, since (taking $\left\|v_{j}\right\|=1$ with negligible error), $\left\|A r_{k}\right\|^{2}=\phi_{k}^{2}\left(\left[\gamma_{k+1}\right]^{2}+2 \gamma_{k+1} \delta_{k+2} v_{k+1}^{T} v_{k+2}+\left[\delta_{k+2}\right]^{2}\right)$, where from (3.7) $\left|\delta_{k+2}\right| \leq \beta_{k+2}$, while from $[38,(18)] \beta_{k+2}\left|v_{k+1}^{T} v_{k+2}\right| \leq O(\varepsilon)\|A\|$, and with $\left|\gamma_{k+1}\right| \leq\|A\|$, see $[38,(19)]$, we see that $\left|\gamma_{k+1} \delta_{k+2} v_{k+1}^{T} v_{k+2}\right| \leq O(\varepsilon)\|A\|^{2}$.

Typically $\left\|A r_{k}\right\|$ is not monotonic, while clearly $\left\|r_{k}\right\|$ and $\left\|A x_{k}\right\|$ are monotonic. In the eigensystem $A=U \Lambda U^{T}$, let $U=\left[\begin{array}{ll}U_{1} & U_{2}\end{array}\right]$, where the eigenvectors $U_{1}$ correspond to nonzero eigenvalues. Then $P_{A} \equiv U_{1} U_{1}^{T}$ and $P_{A}^{\perp} \equiv U_{2} U_{2}^{T}$ are orthogonal projectors [53] onto the range and nullspace of $A$. For general linear LS problems, Chang et al. [7] characterize the dynamics of $\left\|r_{k}\right\|$ and $\left\|A^{T} r_{k}\right\|$ in three phases defined in terms of the ratios among $\left\|r_{k}\right\|,\left\|P_{A} r_{k}\right\|$, and $\left\|P_{A}^{\perp} r_{k}\right\|$, and propose two new stopping criteria for iterative solvers. The expositions $[1,26]$ show that these estimates are cheaply computable in CGLS and LSQR [40, 41].
3.5. Effects of rounding errors in MINRES. MINRES should stop if $R_{k}$ is singular (which theoretically implies $k=\ell$ and $A$ is singular). Singularity was not discussed by Paige and Saunders [39], but they did raise the question: Is MINRES stable when $R_{k}$ is ill-conditioned? Their concern was that $\left\|D_{k}\right\|$ could be large in (3.8), and there could then be cancellation in forming $x_{k-1}+\tau_{k} d_{k}$ in (3.4).

Sleijpen, Van der Vorst, and Modersitzki [47] analyzed the effects of rounding errors in MINRES and reported examples of apparent failure with a matrix of the form $A=Q D Q^{T}$, where $D$ is an ill-conditioned diagonal matrix and $Q$ involves a single plane rotation. We were unable to reproduce MINRES's performance on the two examples defined in Figure 4 of their paper, but we modified the examples by using an $n \times n$ Householder transformation for $Q$, and then observed similar difficulties with MINRES-see Figure 8.2. The recurred residual norm $\phi_{k}^{M}$ is a good approximation to the directly computed $\left\|r_{k}^{M}\right\|$ until the last few iterations. The recurred norms $\phi_{k}^{M}$ then keep decreasing but the directly computed norms $\left\|r_{k}^{M}\right\|$ become stagnant or even increase (see the lower subplots in Figure 8.2).

Remark 3.3. Note that we do want $\phi_{k}$ to keep decreasing on compatible systems, so that the test $\phi_{k} \leq \operatorname{tol}\left(\|A\|\left\|x_{k}\right\|+\|b\|\right)$ with tol $\geq \varepsilon$ will eventually be satisfied even if the computed $\left\|r_{k}\right\|$ is no longer as small as $\phi_{k}$.

The analysis in [47] focuses on the rounding errors involved in the $n$ lower triangular solves $R_{k}^{T} D_{k}^{T}=V_{k}^{T}$ (one solve for each row of $D_{k}$ ), compared to the single upper triangular solve $R_{k} y_{k}=t_{k}$ (followed by $x_{k}=V_{k} y_{k}$ ) that would be possible at the final $k$ if all of $V_{k}$ were stored as in GMRES [44]. We shall see that a key feature of MINRES-QLP is that a single lower triangular solve suffices with no need to store $V_{k}$, much the same as in SYMMLQ.
4. Orthogonal decompositions for singular matrices. In 1999 Stewart proposed the pivoted $Q L P$ decomposition [51], which is equivalent to two consecutive QR factorizations with column interchanges, first on $A$, then on $R^{T}$ :

$$
Q_{R} A \Pi_{R}=\left[\begin{array}{cc}
R & S  \tag{4.1}\\
0 & 0
\end{array}\right], \quad Q_{L}\left[\begin{array}{cc}
R^{T} & 0 \\
S^{T} & 0
\end{array}\right] \Pi_{L}=\left[\begin{array}{cc}
\hat{R} & 0 \\
0 & 0
\end{array}\right]
$$

giving nonnegative diagonal elements, where $\Pi_{R}$ and $\Pi_{L}$ are permutations chosen to maximize the next diagonal element of $R$ and $\hat{R}$ at each stage. This gives $A=Q L P$, where

$$
Q=Q_{R}^{T} \Pi_{L}, \quad L=\left[\begin{array}{cc}
\hat{R}^{T} & 0 \\
0 & 0
\end{array}\right], \quad P=Q_{L} \Pi_{R}^{T}
$$

with $Q$ and $P$ orthogonal. Stewart demonstrated that the diagonals of $L$ (the $L$ values) give better singular-value estimates than the diagonals of $R$ (the $R$-values), and the accuracy is particularly good for the extreme singular values $\sigma_{1}$ and $\sigma_{n}$ :

$$
\begin{equation*}
R_{i i} \approx \sigma_{i}, \quad L_{i i} \approx \sigma_{i}, \quad \sigma_{1} \geq \max _{i} L_{i i} \geq \max _{i} R_{i i}, \quad \min _{i} R_{i i} \geq \min _{i} L_{i i} \geq \sigma_{n} \tag{4.2}
\end{equation*}
$$

The first permutation $\Pi_{R}$ in pivoted QLP is important. The main purpose of the second permutation $\Pi_{L}$ is to ensure that the $L$-values present themselves in decreasing order, which is not always necessary. If $\Pi_{R}=\Pi_{L}=I$, it is simply called the $Q L P$ decomposition.
5. MINRES-QLP. We now develop MINRES-QLP for solving ill-conditioned or singular symmetric systems $A x \approx b$. The Lanczos framework is the same as in MINRES, but we handle $T_{\ell}$ in (3.5) with extra care when it is rank-deficient. In this case, the normal approach to solving (3.5) is via a QLP decomposition of $T_{\ell}$ to obtain the (unique) minimum-length solution $y_{\ell}[51,18]$. Thus in MINRES-QLP we use a QLP decomposition of $\underline{T_{k}}$ in subproblem (3.2) for all $k \leq \ell$. This is the MINRES QR (3.3) followed by an LQ factorization of $R_{k}$ :

$$
Q_{k} \underline{T_{k}}=\left[\begin{array}{c}
R_{k}  \tag{5.1}\\
0
\end{array}\right], \quad R_{k} P_{k}=L_{k}, \quad \text { so that } \quad Q_{k} \underline{T_{k}} P_{k}=\left[\begin{array}{c}
L_{k} \\
0
\end{array}\right]
$$

where $Q_{k}$ and $P_{k}$ are orthogonal, $R_{k}$ is upper tridiagonal and $L_{k}$ is lower tridiagonal. When $k<\ell, R_{k}$ and $L_{k}$ are nonsingular. MINRES-QLP obtains the same solution as MINRES, but by a different process (and with different rounding errors). Defining $u$ by $y=P_{k} u$, we see from (3.3) that

$$
Q_{k}\left(\underline{T_{k}} y-\beta_{1} e_{1}\right)=\left[\begin{array}{c}
L_{k} \\
0
\end{array}\right] u-\left[\begin{array}{c}
t_{k} \\
\phi_{k}
\end{array}\right]
$$

and (3.2) is solved by $L_{k} u_{k}=t_{k}$ and $y_{k}=P_{k} u_{k}$. The MINRES-QLP estimate of $x$ is therefore $x_{k}=V_{k} y_{k}=V_{k} P_{k} u_{k}=W_{k} u_{k}$, with theoretically orthonormal $W_{k} \equiv V_{k} P_{k}$.

We will see that only the last three columns of $V_{k}$ are needed to update $x_{k}$.
5.1. The QLP factorization of $\underline{T_{k}}$. The QLP decomposition of each $\underline{T_{k}}$ must be without permutations in order to ensure inexpensive updating of the factors as $k$ increases. Our experience is that the desired rank-revealing properties (4.2) tend to be retained, perhaps because of the tridiagonal structure of $\underline{T_{k}}$ and the convergence properties of the underlying Lanczos process.

For $k<\ell$, the QLP decomposition of $\underline{T_{k}}$ (5.1) gives nonsingular tridiagonal $R_{k}$ and $L_{k}$. As in MINRES, $Q_{k}$ is a product of Householder reflectors, see (3.3) and (3.7), while $P_{k}$ involves a product of pairs of essentially $2 \times 2$ reflectors:

$$
Q_{k}=Q_{k, k+1} \cdots Q_{3,4} \quad Q_{2,3} \quad Q_{1,2}, \quad P_{k}=P_{1,2} \quad P_{1,3} P_{2,3} \cdots P_{k-2, k} P_{k-1, k} .
$$

For MINRES-QLP to be efficient, in the $k$ th iteration $(k \geq 3)$ the application of the left reflector $Q_{k, k+1}$ is followed immediately by the right reflectors $P_{k-2, k}, P_{k-1, k}$, so that only the last $2 \times 2$ principal submatrix of the transformed $\underline{T_{k}}$ will be changed in future iterations. These ideas can be understood more easily from Figure 5.1 and the following compact form, which represents the actions of right reflectors on $\underline{T_{k}}$ (additional to $Q_{k, k+1}(3.7)$ ):

$$
\left.\begin{array}{rl} 
& {\left[\begin{array}{lll}
\gamma_{k-2}^{(5)} & & \epsilon_{k} \\
\vartheta_{k-1} & \gamma_{k-1}^{(4)} & \delta_{k}^{(2)} \\
= & & \gamma_{k}^{(2)}
\end{array}\right]\left[\begin{array}{lll}
c_{k 2} & & s_{k 2} \\
& 1 & \\
s_{k 2} & & -c_{k 2}
\end{array}\right]\left[\begin{array}{lll}
1 & & \\
& c_{k 3} & s_{k 3} \\
& s_{k 3} & -c_{k 3}
\end{array}\right]} \\
\vartheta_{k-1}^{(2)} & \gamma_{k-1}^{(4)}  \tag{5.2}\\
\eta_{k} & \delta_{k}^{(3)} \\
\gamma_{k-2}^{(6)} & \gamma_{k}^{(3)}
\end{array}\right]\left[\begin{array}{ccc}
1 & & \\
& c_{k 3} & s_{k 3} \\
& s_{k 3} & -c_{k 3}
\end{array}\right]=\left[\begin{array}{ccc}
\gamma_{k-2}^{(6)} & \\
\vartheta_{k-1}^{(2)} & \gamma_{k-1}^{(5)} & \\
\eta_{k} & \vartheta_{k} & \gamma_{k}^{(4)}
\end{array}\right] .
$$

5.2. The diagonals of $L_{k}$. Figure 5.2 shows the relation between the singular values of $A$ and the diagonal elements of $R_{k}$ and $L_{k}$ with $k=19$. This illustrates (4.2) for matrix ID 1177 from [54] with $n=25$.


FIG. 5.1. QLP with left and right reflectors interleaved on $T_{5}$. This figure can be reproduced with the help of QLPfig5.m.


Fig. 5.2. Upper left: Nonzero singular values of A sorted in decreasing order. Upper middle and right: The diagonals $\gamma_{k}^{M}$ of $R_{k}$ (red circles) from MINRES are plotted as red circles above or below the nearest singular value of $A$. They approximate the extreme nonzero singular values of $A$ well. Lower: The diagonals $\gamma_{k}^{Q}$ of $L_{k}$ (red circles) from MINRES-QLP approximate the extreme nonzero singular values of $A$ even better. An implication is that the ratio of the largest and smallest diagonals of $L_{k}$ provides a good estimate of $\kappa(A)$. To reproduce this figure, run test_minresqlp_fig3(2).
5.3. Solving the subproblem. With $y_{k}=P_{k} u_{k}$, subproblem (3.2) becomes

$$
u_{k}=\arg \min _{u \in \mathbb{R}^{k}}\left\|\left[\begin{array}{c}
L_{k}  \tag{5.3}\\
0
\end{array}\right] u-\left[\begin{array}{c}
t_{k} \\
\phi_{k}
\end{array}\right]\right\|,
$$

where $t_{k}$ and $\phi_{k}$ are as in (3.3) and (3.6). At the start of iteration $k$, the first $k-3$ elements of $u_{k}$, denoted by $\mu_{j}$ for $j \leq k-3$, are known from previous iterations; see the 10th matrix in Figure 5.1. The remainder depend on the rank of $L_{k}$.

1. If $\operatorname{rank}\left(L_{k}\right)=k$ (so $k<\ell$, or $k=\ell$ and $b \in \operatorname{range}(A)$ ), we need to solve the last three equations of $L_{k} u_{k}=t_{k}$ :

$$
\left[\begin{array}{ccc}
\gamma_{k-2}^{(6)} & &  \tag{5.4}\\
\vartheta_{k-1}^{(2)} & \gamma_{k-1}^{(5)} & \\
\eta_{k} & \vartheta_{k} & \gamma_{k}^{(4)}
\end{array}\right]\left[\begin{array}{c}
\mu_{k-2}^{(3)} \\
\mu_{k-1}^{(2)} \\
\mu_{k}
\end{array}\right]=\left[\begin{array}{c}
\bar{\tau}_{k-2} \\
\bar{\tau}_{k-1} \\
\tau_{k}
\end{array}\right] \equiv\left[\begin{array}{c}
\tau_{k-2}-\eta_{k-2} \mu_{k-4}^{(4)}-\vartheta_{k-2} \mu_{k-3}^{(3)} \\
\tau_{k-1}-\eta_{k-1} \mu_{k-3}^{(3)} \\
\tau_{k}
\end{array}\right]
$$

2. If $k=\ell$ and $b \notin \operatorname{range}(A)$, the last row and column of $L_{k}$ are zero, and we only need to solve the last two equations of $L_{k-1} u_{k-1}=t_{k-1}$, where

$$
L_{k}=\left[\begin{array}{cc}
L_{k-1} &  \tag{5.5}\\
0 & 0
\end{array}\right], \quad u_{k}=\left[\begin{array}{c}
u_{k-1} \\
0
\end{array}\right], \quad\left[\begin{array}{ll}
\gamma_{k-2}^{(6)} & \\
\vartheta_{k-1}^{(2)} & \gamma_{k-1}^{(5)}
\end{array}\right]\left[\begin{array}{l}
\mu_{k-2}^{(3)} \\
\mu_{k-1}^{(2)}
\end{array}\right]=\left[\begin{array}{c}
\bar{\tau}_{k-2} \\
\bar{\tau}_{k-1}
\end{array}\right]
$$

The corresponding solution estimate is $x_{k}=V_{k} y_{k}=V_{k} P_{k} u_{k}=W_{k} u_{k}$, where

$$
\begin{align*}
W_{k} \equiv V_{k} P_{k} & =\left[\begin{array}{llll}
V_{k-1} P_{k-1} & v_{k}
\end{array}\right] P_{k-2, k} P_{k-1, k}  \tag{5.6}\\
& =\left[\begin{array}{llll}
W_{k-3}^{(4)} & w_{k-2}^{(3)} & w_{k-1}^{(2)} & v_{k}
\end{array}\right] P_{k-2, k} P_{k-1, k} \\
& =\left[\begin{array}{llll}
W_{k-3}^{(4)} & w_{k-2}^{(4)} & w_{k-1}^{(3)} & w_{k}^{(2)}
\end{array}\right] \\
W_{k}^{T} W_{k} & =I_{k}, \quad \operatorname{range}\left(W_{k}\right)=\mathcal{K}_{k}(A, b) \tag{5.7}
\end{align*}
$$

and we update $x_{k-2}$ and compute $x_{k}$ by short-recurrence orthogonal steps:

$$
\begin{align*}
x_{k-2}^{(2)} & =x_{k-3}^{(2)}+w_{k-2}^{(4)} \mu_{k-2}^{(3)}, \text { where } x_{k-3}^{(2)} \equiv W_{k-3}^{(4)} u_{k-3}^{(3)},  \tag{5.8}\\
x_{k} & =x_{k-2}^{(2)}+w_{k-1}^{(3)} \mu_{k-1}^{(2)}+w_{k}^{(2)} \mu_{k} . \tag{5.9}
\end{align*}
$$

5.4. Termination. When $k=\ell, Q_{k, k+1}$ is not formed or applied, see (3.3) and (3.7), and the QR factorization stops. In MINRES-QLP, we still need to apply $P_{k-2, k} P_{k-1, k}$ on the right to obtain the minimum-length solution; see Figure 5.1.

Theorem 5.1 ([10, Theorem 3.1]). In MINRES-QLP, $x_{\ell}=x^{\dagger}$.
Proof. When $b \in \operatorname{range}(A)$, the proof is the same as that for Theorem 3.1.
When $b \notin \operatorname{range}(A)$, for all $u=\left[\begin{array}{ll}u_{\ell-1} & \mu_{k}\end{array}\right]^{T} \in \mathbb{R}^{\ell}$ that solves (5.3), MINRES-QLP returns the min-length LS solution $u_{\ell}=\left[\begin{array}{ll}u_{\ell-1} & 0\end{array}\right]^{T}$ by the construction in (5.5). For any $x \in \operatorname{range}\left(W_{\ell}\right)=\mathcal{K}_{\ell}(A, b)$ by (5.7),

$$
\begin{aligned}
\|A x-b\| & =\left\|A W_{\ell} u-b\right\|=\left\|A V_{\ell} P_{\ell} u-b\right\|=\left\|V_{\ell} T_{\ell} P_{\ell} u-\beta_{1} V_{\ell} e_{1}\right\|=\left\|T_{\ell} P_{\ell} u-\beta_{1} e_{1}\right\| \\
& =\left\|Q_{\ell-1} T_{\ell} P_{\ell} u-\left[\begin{array}{c}
t_{\ell-1} \\
\phi_{\ell-1}
\end{array}\right]\right\|=\left\|\left[\begin{array}{cc}
L_{\ell-1} & 0 \\
0 & 0
\end{array}\right] u-\left[\begin{array}{c}
t_{\ell-1} \\
\phi_{\ell-1}
\end{array}\right]\right\| .
\end{aligned}
$$

Since $L_{\ell-1}$ is nonsingular, $\phi_{\ell-1}=\min \|A x-b\|$ can be achieved by $x_{\ell}=W_{\ell} u_{\ell}=$ $W_{\ell-1} u_{\ell-1}$ and $\left\|x_{\ell}\right\|=\left\|W_{\ell-1} u_{\ell-1}\right\|=\left\|u_{\ell-1}\right\|$ by (5.7). Thus $x_{\ell}$ is the min-length LS
solution of $\|A x-b\|$ in $\mathcal{K}_{\ell}(A, b)$, i.e., $x_{\ell}=\arg \min \left\{\|x\| \mid A^{2} x=A b, x \in \mathcal{K}_{\ell}(A, b)\right\}$. Likewise $y_{\ell}=P_{\ell} u_{\ell}$ is the min-length LS solution of $\left\|T_{\ell} y-\beta_{1} e_{1}\right\|$ and so $y_{\ell} \in \operatorname{range}\left(T_{\ell}\right)$, i.e. $y_{\ell}=T_{\ell} z$ for some $z$. Thus $x_{\ell}=V_{\ell} y_{\ell}=V_{\ell} T_{\ell} z=A V_{\ell} z \in \operatorname{range}(A)$. We know that $x^{\dagger}=\arg \min \left\{\|x\| \mid A^{2} x=A b, x \in \mathbb{R}^{n}\right\}$ is unique and $x^{\dagger} \in \operatorname{range}(A)$. Since $x_{\ell} \in \operatorname{range}(A)$, we must have $x_{\ell}=x^{\dagger}$.
5.5. Transfer from MINRES to MINRES-QLP. On well-conditioned systems, MINRES and MINRES-QLP behave very similarly. However, MINRES-QLP requires one more vector of storage, and each iteration needs 4 more axpy's $(y \leftarrow \alpha x+y)$ and 3 more vector scalings $(x \leftarrow \alpha x)$. Thus it would be a desirable feature to invoke MINRES-QLP from MINRES only if $A$ is ill-conditioned or singular. The key idea is to transfer to MINRES-QLP at an iteration where $T_{k}$ is not yet too ill-conditioned. The MINRES and MINRES-QLP solution estimates are the same, so from (3.4), (5.9), and (5.3): $x_{k}^{M}=x_{k} \Longleftrightarrow D_{k} t_{k}=W_{k} u_{k}=W_{k} L_{k}^{-1} t_{k}$. Now from (3.8), (5.1), and (5.6),

$$
\begin{equation*}
D_{k} L_{k}=\left(V_{k} R_{k}^{-1}\right)\left(R_{k} P_{k}\right)=V_{k} P_{k}=W_{k}, \tag{5.10}
\end{equation*}
$$

and the last three columns of $W_{k}$ can be obtained from the last three columns of $D_{k}$ and $L_{k}$. (Thus, we transfer the three MINRES basis vectors $d_{k-2}, d_{k-1}, d_{k}$ to $w_{k-2}, w_{k-1}, w_{k}$.) In addition, we need to generate $x_{k-2}^{(2)}$ using (5.8):

$$
x_{k-2}^{(2)}=x_{k}^{M}-w_{k-1}^{(3)} \mu_{k-1}^{(2)}-w_{k}^{(2)} \mu_{k} .
$$

It is clear from (5.10) that we still need to do the right transformation $R_{k} P_{k}=L_{k}$ in the MINRES phase and keep the last $3 \times 3$ principal submatrix of $L_{k}$ for each $k$ so that we are ready to transfer to MINRES-QLP when necessary. We then obtain a short recurrence for $\left\|x_{k}\right\|$ (see section 6.5) and for this computation we save flops relative to the original MINRES algorithm, where $\left\|x_{k}\right\|$ is computed directly.

In the implementation, the MINRES iterates transfer to MINRES-QLP iterates when an estimate of the condition number of $T_{k}$ (see (6.3)) exceeds an input parameter trancond. Thus, trancond $>1 / \varepsilon$ leads to MINRES iterates throughout, while trancond $=1$ generates MINRES-QLP iterates from the start.
5.6. Comparison of Lanczos-based solvers. We compare MINRES-QLP with CG, SYMMLQ, and MINRES in Tables 5.1-5.2 in terms of subproblem definitions, basis, solution estimates, flops and memory. A careful implementation of SYMMLQ provides a point in $\mathcal{K}_{k+1}(A, b)$ as shown. All solvers need storage for $v_{k}, v_{k+1}, x_{k}$, and a product $p_{k}=A v_{k}$ each iteration. Some additional work-vectors are needed for each method (e.g., $d_{k-1}$ and $d_{k}$ for MINRES, giving 7 work-vectors in total).
6. Stopping conditions and norm estimates. This section derives several norm estimates that are computed in MINRES-QLP. As before, we assume exact arithmetic throughout, so that $V_{k}$ and $Q_{k}$ are orthonormal. Table 6.1 summarizes how the norm estimates are used to formulate three groups of stopping conditions. The second NRBE test $\left\|A r_{k}\right\| \leq\|A\|\left\|r_{k}\right\| t o l$ is from Stewart [50] with symmetric $A$.
6.1. Residual and residual norm. First we derive recurrence relations for $r_{k}$ and its norm $\phi_{k} \equiv\left\|r_{k}\right\|$.

Lemma $6.1\left(r_{k}\right.$ and $\left\|r_{k}\right\|$ for MINRES-QLP and monotonicity of $\left.\left\|r_{k}\right\|\right)$.

- If $k<\ell$, then $\operatorname{rank}\left(L_{k}\right)=k, r_{k}=s_{k}^{2} r_{k-1}-\phi_{k} c_{k} v_{k+1}$, and $\phi_{k}=\phi_{k-1} s_{k}>0$.
- If $\operatorname{rank}\left(L_{\ell}\right)=\ell$, then $r_{\ell}=0$.
- If $\operatorname{rank}\left(L_{\ell}\right)=\ell-1$, then $r_{\ell}=r_{\ell-1} \neq 0$, and $\left\|r_{\ell}\right\|=\phi_{\ell-1}>0$.

TABLE 5.1
Subproblems defining $x_{k}$ for $C G$, SYMMLQ, MINRES, and MINRES-QLP.

| Method | Subproblem | Factorization | Estimate of $x_{k}$ |
| :---: | :---: | :---: | :---: |
| $\begin{aligned} & \hline \text { cgLanczos } \\ & {[24,39,48]} \end{aligned}$ | $T_{k} y_{k}=\beta_{1} e_{1}$ | Cholesky: $T_{k}=L_{k} D_{k} L_{k}^{T}$ | $\begin{aligned} & x_{k}^{C}=V_{k} y_{k} \\ & \quad \in \mathcal{K}_{k}(A, b) \end{aligned}$ |
| $\begin{aligned} & \text { SYMMLQ } \\ & {[39,45]} \end{aligned}$ | $\begin{aligned} & y_{k+1}=\arg \min _{y \in \mathbb{R}^{k+1}}\\|y\\| \\ & \quad \text { s.t. } T_{k}^{T} y=\beta_{1} e_{1} \end{aligned}$ | LQ: <br> ${\underline{T_{k}}}^{T} Q_{k}^{T}=\left[\begin{array}{ll}L_{k} & 0\end{array}\right]$ | $\begin{aligned} & x_{k}^{L}=V_{k+1} y_{k+1} \\ & \quad \in \mathcal{K}_{k+1}(A, b) \end{aligned}$ |
| MINRES [39] | $y_{k}=\arg \min _{y \in \mathbb{R}^{k}}\left\\|\underline{T_{k}} y-\beta_{1} e_{1}\right\\|$ | QR: $Q_{k} \underline{T_{k}}=\left[\begin{array}{c} R_{k} \\ 0 \end{array}\right]$ | $\begin{aligned} & x_{k}^{M}=V_{k} y_{k} \\ & \quad \in \mathcal{K}_{k}(A, b) \end{aligned}$ |
| $\begin{aligned} & \text { MINRES-QLP } \\ & {[10]} \end{aligned}$ | $\begin{aligned} & y_{k}=\arg \min _{y \in \mathbb{R}^{k}}\\|y\\| \\ & \text { s.t. } y \in \arg \min \left\\|\underline{T_{k}} y-\beta_{1} e_{1}\right\\| \end{aligned}$ | QLP: $Q_{k} \underline{T_{k}} P_{k}=\left[\begin{array}{c} L_{k} \\ 0 \end{array}\right]$ | $\begin{aligned} & x_{k}^{Q}=V_{k} y_{k} \\ & \quad \in \mathcal{K}_{k}(A, b) \end{aligned}$ |

Table 5.2
Bases, subproblem solutions, storage, and work for each method.

| Method | New basis | $z_{k}, t_{k}, u_{k}$ | $x_{k}$ estimate | vecs | flops |
| :--- | :--- | :---: | :--- | :--- | :--- |
| cgLanczos | $W_{k} \equiv V_{k} L_{k}^{-T}$ | $L_{k} D_{k} z_{k}=\beta_{1} e_{1}$ | $x_{k}^{C}=W_{k} z_{k}$ | 5 | $8 n$ |
| SYMMLQ | $W_{k} \equiv V_{k+1} Q_{k}^{T}\left[\begin{array}{c}I_{k} \\ 0\end{array}\right]$ | $L_{k} z_{k}=\beta_{1} e_{1}$ | $x_{k}^{L}=W_{k} z_{k}$ | 6 | $9 n$ |
| MINRES | $D_{k} \equiv V_{k} R_{k}^{-1}$ | $t_{k}=\beta_{1}\left[\begin{array}{ll}I_{k} & 0\end{array}\right] Q_{k} e_{1}$ | $x_{k}^{M}=D_{k} t_{k}$ | 7 | $9 n$ |
| MINRES-QLP | $W_{k} \equiv V_{k} P_{k}$ | $L_{k} u_{k}=\beta_{1}\left[\begin{array}{ll}I_{k} & 0\end{array}\right] Q_{k} e_{1}$ | $x_{k}^{Q}=W_{k} u_{k}$ | 8 | $14 n$ |

Proof. If $k<\ell$, the residual is the same as for MINRES. We have $\left\|r_{k}\right\|=\phi_{k}=$ $\phi_{k-1} s_{k}>0$; see (3.6)-(3.9). Also from $r_{k}=\phi_{k} V_{k+1} Q_{k}^{T} e_{k+1}$ (3.10) we have

$$
\begin{aligned}
r_{k} & =\phi_{k}\left[\begin{array}{ll}
V_{k} & v_{k+1}
\end{array}\right]\left[\begin{array}{ll}
Q_{k-1}^{T} & \\
& 1
\end{array}\right]\left[\begin{array}{lll}
I_{k-1} & & \\
& c_{k} & s_{k} \\
& s_{k} & -c_{k}
\end{array}\right]\left[\begin{array}{l}
0 \\
0 \\
1
\end{array}\right] \quad \text { by }(3.3), \\
& =\phi_{k}\left[\begin{array}{ll}
V_{k} & v_{k+1}
\end{array}\right]\left[\begin{array}{ll}
Q_{k-1}^{T} & \\
& 1
\end{array}\right]\left[\begin{array}{c}
s_{k} e_{k} \\
-c_{k}
\end{array}\right]=\phi_{k}\left[\begin{array}{ll}
V_{k} & v_{k+1}
\end{array}\right]\left[\begin{array}{c}
s_{k} Q_{k-1}^{T} e_{k} \\
-c_{k}
\end{array}\right] \\
& =\phi_{k} s_{k} V_{k} Q_{k-1}^{T} e_{k}-\phi_{k} c_{k} v_{k+1}=\phi_{k-1} s_{k}^{2} V_{k} Q_{k-1}^{T} e_{k}-\phi_{k} c_{k} v_{k+1} \\
& =s_{k}^{2} r_{k-1}-\phi_{k} c_{k} v_{k+1} \text { by (3.10). }
\end{aligned}
$$

If $T_{\ell}$ is nonsingular, $r_{\ell}=0$. Otherwise $Q_{\ell-1, \ell}$ has made the last row of $R_{\ell}$ zero, so the last row and column of $L_{\ell}$ are zero; see (5.5). Thus $r_{\ell}=r_{\ell-1} \neq 0$; see Remark 3.2. प
6.2. Norm of $A r_{k}$. Next we derive recurrence relations for $A r_{k}$ and its norm $\psi_{k} \equiv\left\|A r_{k}\right\|$, and we show that $A r_{k}$ is orthogonal to $\mathcal{K}_{k}(A, b)$.

LEmma $6.2\left(A r_{k}\right.$ and $\psi_{k} \equiv\left\|A r_{k}\right\|$ for MINRES-QLP).

- If $k<\ell$, then $\operatorname{rank}\left(L_{k}\right)=k, A r_{k}=\left\|r_{k}\right\|\left(\gamma_{k+1} v_{k+1}+\delta_{k+2} v_{k+2}\right)$ and $\psi_{k}=$ $\left\|r_{k}\right\|\left\|\left[\begin{array}{ll}\gamma_{k+1} & \delta_{k+2}\end{array}\right]\right\|$, where $\delta_{k+2}=0$ if $k=\ell-1$.
- If $\operatorname{rank}\left(L_{\ell}\right)=\ell$, then $A r_{\ell}=0$ and $\psi_{\ell}=0$.
- If $\operatorname{rank}\left(L_{\ell}\right)=\ell-1$, then $A r_{\ell}=A r_{\ell-1}=0$, and $\left\|\psi_{\ell}\right\|=\psi_{\ell-1}=0$.

Proof. For the first case, the proof is essentially the same as the proof of Lemma 3.3. For the other two cases, the results follow directly from Lemma 6.1.

TABLE 6.1
Stopping conditions in MINRES-QLP. NRBE means normwise relative backward error, and tol, maxit, maxcond, and maxxnorm are input parameters. All norms and $\kappa(A)$ are estimated by MINRES-QLP.

| Lanczos | NRBE | Regularization attempts |
| :--- | :--- | :--- |
| $\beta_{k+1} \leq n\\|A\\| \varepsilon$ | $\left\\|r_{k}\right\\| /\left(\\|A\\|\left\\|x_{k}\right\\|+\\|b\\|\right) \leq$ tol | $\kappa(A) \geq$ maxcond |
| $k=$ maxit | $\left\\|A r_{k}\right\\| /\left(\\|A\\|\left\\|r_{k}\right\\|\right) \leq$ tol | $\left\\|x_{k}\right\\| \geq$ maxxnorm |

6.3. Matrix norms. For Lanczos-based algorithms, $\|A\| \geq\left\|V_{k+1}^{T} A V_{k}\right\|=\left\|\underline{T_{k}}\right\|$. Define

$$
\begin{equation*}
\mathcal{A}^{(0)} \equiv 0, \quad \mathcal{A}^{(k)} \equiv \max _{j=1, \ldots, k}\left\{\left\|\underline{T_{j}} e_{j}\right\|\right\}=\max \left\{\mathcal{A}^{(k-1)},\left\|\underline{T_{k}} e_{k}\right\|\right\} \text { for } k \geq 1 \tag{6.1}
\end{equation*}
$$

Then $\|A\| \geq\left\|\underline{T_{k}}\right\| \geq \mathcal{A}^{(k)}$. Clearly, $\mathcal{A}^{(k)}$ is monotonically increasing and is thus an improving estimate for $\|A\|$ as $k$ increases. By the property of QLP decomposition in (4.2) and (5.2), we could easily extend (6.1) to include the largest diagonal of $L_{k}$ :

$$
\begin{equation*}
\mathcal{A}^{(0)} \equiv 0, \quad \mathcal{A}^{(k)} \equiv \max \left\{\mathcal{A}^{(k-1)},\left\|\underline{T_{k}} e_{k}\right\|, \gamma_{k-2}^{(6)}, \gamma_{k-1}^{(5)},\left|\gamma_{k}^{(4)}\right|\right\} \text { for } k \geq 1 \tag{6.2}
\end{equation*}
$$

Some other schemes inspired by Larsen [31, section A.6.1], Higham [25], and Chen and Demmel [8] follow. For the latter scheme, we use an implementation by Kaustuv [28] for estimating the norms of the rows of $A$.

1. $[31]\left\|T_{k}\right\|_{1} \geq\left\|T_{k}\right\|$
2. $[31] \sqrt{\| \underline{T_{k}}}{ }^{T} \underline{T_{k}}\left\|_{1} \geq\right\| T_{k} \|$
3. [31] $\left\|T_{j}\right\| \leq\left\|T_{k}\right\|$ for small $j=5$ or 20
4. [25] Matlab function $\operatorname{NORMEST}(A)$, which is based on the power method
5. [8] $\max _{i}\left\|h_{i}\right\| / \sqrt{m}$, where $h_{i}^{T}$ is the $i$ th row of $A Z$, each column of $Z \in \mathbb{R}^{n \times m}$ is a random vector of $\pm 1$ 's, and $m$ is a small integer (e.g., $m=10$ ).
Figure 6.1 plots estimates of $\|A\|$ for 12 matrices from the Florida sparse matrix collection [54] whose sizes $n$ vary from 25 to 3002 . In particular, scheme 3 above with $j=20$ gives significantly more accurate estimates than other schemes for the 12 matrices we tried. However, the choice of $j$ is not always clear and the scheme adds a little to the cost of MINRES-QLP. Hence we propose incorporating it into MINRES-QLP (or other Lanzcos-based iterative methods) if very accurate $\|A\|$ is needed. Otherwise (6.2) uses quantities readily available from MINRES-QLP and gives us satisfactory estimates for the order of $\|A\|$.
6.4. Matrix condition numbers. We again apply the property of the QLP decomposition in (4.2) and (5.2) to estimate $\kappa\left(\underline{T_{k}}\right)$, which is a lower bound for $\kappa(A)$ :

$$
\begin{align*}
& \gamma_{\min } \leftarrow \min \left\{\gamma_{1}, \gamma_{2}^{(2)}\right\}, \quad \gamma_{\min } \leftarrow \min \left\{\gamma_{\min }, \gamma_{k-2}^{(6)}, \gamma_{k-1}^{(5)},\left|\gamma_{k}^{(4)}\right|\right\} \text { for } k \geq 3 \\
& \kappa^{(0)} \equiv 1, \quad \kappa^{(k)} \equiv \max \left\{\kappa^{(k-1)}, \frac{\mathcal{A}^{(k)}}{\gamma_{\min }}\right\} \text { for } k \geq 1 \tag{6.3}
\end{align*}
$$

6.5. Solution norms. We derive a recurrence relation for $\left\|x_{k}\right\|$ whose cost is as low as computing the norm of a 3 - or 4- vector.

Since $\left\|x_{k}\right\|=\left\|V_{k} P_{k} u_{k}\right\|=\left\|u_{k}\right\|$, we can estimate $\left\|x_{k}\right\|$ by computing $\chi_{k} \equiv\left\|u_{k}\right\|$. However, the last two elements of $u_{k}$ change in $u_{k+1}$ (and a new element $\mu_{k+1}$ is


Fig. 6.1. Relative errors in different estimates of $\|A\|$. This figure can be reproduced by testminresQLPNormA8.
added). We therefore maintain $\chi_{k-2}$ by updating it and then using it according to

$$
\chi_{k-2}^{(2)}=\left\|\left[\begin{array}{ll}
\chi_{k-3}^{(2)} & \mu_{k-2}^{(3)}
\end{array}\right]\right\|, \quad \chi_{k}=\left\|\left[\begin{array}{lll}
\chi_{k-2}^{(2)} & \mu_{k-1}^{(2)} & \mu_{k}
\end{array}\right]\right\| \quad \text { cf. (5.8) and (5.9). }
$$

Thus $\chi_{k-2}^{(2)}$ increases monotonically but we cannot guarantee that $\left\|x_{k}\right\|$ and its recurred estimate $\chi_{k}$ are increasing, and indeed they are not in some examples (see Figure 8.1).
6.6. Projection norms. Sometimes the projection of the right-hand side vector $b$ onto $\mathcal{K}_{k}(A, b)$ is required (for example, see [46]). A simple recurrence relation is $\omega_{k}^{2} \equiv\left\|A x_{k}\right\|^{2}=\omega_{k-1}^{2}+\tau_{k}^{2}$ and we can derive it in the same way as shown in Lemma 3.3. With $\omega_{0} \equiv 0$ we have $\omega_{k} \equiv\left\|A x_{k}\right\|=\left\|\left[\begin{array}{ll}\omega_{k-1} & \tau_{k}\end{array}\right]\right\|$.
7. Preconditioned MINRES and MINRES-QLP. It is often asked: How can we construct a preconditioner for a linear system solver so that the same problem is solved with fewer iterations? Previous work on preconditioning the symmetric solvers CG, SYMMLQ, or MINRES includes $[43,37,17,12,14,35,42,34,20,2,52]$.

We have the same question for singular symmetric systems $A x \approx b$. Two-sided preconditioning is needed to preserve symmetry. We can still solve compatible systems, but we will no longer obtain the minimum-length solution. For incompatible systems, preconditioning alters the "least squares" norm. To avoid this difficulty we must work with larger equivalent systems that are compatible. We consider each case in turn, using a positive-definite preconditioner $M=C C^{T}$ with MINRES and MINRES-QLP to solve symmetric compatible systems $A x=b$. Implicitly, we are solving equivalent symmetric systems $C^{-1} A C^{-T} y=C^{-1} b$, where $C^{T} x=y$. As usual, it is possible to work with $M$ itself, so without loss of generality we can assume $C=M^{\frac{1}{2}}$.
7.1. Derivation. We derive preconditioned MINRES for compatible $A x=b$ by applying MINRES to the equivalent problem $\bar{A} \bar{x}=\bar{b}$, where $\bar{A} \equiv M^{-\frac{1}{2}} A M^{-\frac{1}{2}}$, $\bar{b} \equiv M^{-\frac{1}{2}} b$, and $x=M^{-\frac{1}{2}} \bar{x}$.
7.1.1. Preconditioned Lanczos process. Let $v_{k}$ denote the Lanczos vectors of $\mathcal{K}(\bar{A}, \bar{b})$. With $v_{0}=0$ and $\beta_{1} v_{1}=\bar{b}$, for $k=1,2, \ldots$ we define

$$
\begin{equation*}
z_{k}=\beta_{k} M^{\frac{1}{2}} v_{k}, \quad q_{k}=\beta_{k} M^{-\frac{1}{2}} v_{k}, \quad \text { so that } \quad M q_{k}=z_{k} \tag{7.1}
\end{equation*}
$$

Then $\beta_{k}=\left\|\beta_{k} v_{k}\right\|=\left\|M^{-\frac{1}{2}} z_{k}\right\|=\left\|z_{k}\right\|_{M^{-1}}=\left\|q_{k}\right\|_{M}=\sqrt{q_{k}^{T} z_{k}}$, where the square root is well defined because $M$ is positive definite, and the Lanczos iteration is

$$
\begin{aligned}
p_{k} & =\bar{A} v_{k}=M^{-\frac{1}{2}} A M^{-\frac{1}{2}} v_{k}=M^{-\frac{1}{2}} A q_{k} / \beta_{k} \\
\alpha_{k} & =v_{k}^{T} p_{k}=q_{k}^{T} A q_{k} / \beta_{k}^{2} \\
\beta_{k+1} v_{k+1} & =M^{-\frac{1}{2}} A M^{-\frac{1}{2}} v_{k}-\alpha_{k} v_{k}-\beta_{k} v_{k-1}
\end{aligned}
$$

Multiplying the last equation by $M^{\frac{1}{2}}$ we get

$$
\begin{aligned}
z_{k+1}=\beta_{k+1} M^{\frac{1}{2}} v_{k+1} & =A M^{-\frac{1}{2}} v_{k}-\alpha_{k} M^{\frac{1}{2}} v_{k}-\beta_{k} M^{\frac{1}{2}} v_{k-1} \\
& =\frac{1}{\beta_{k}} A q_{k}-\frac{\alpha_{k}}{\beta_{k}} z_{k}-\frac{\beta_{k}}{\beta_{k-1}} z_{k-1}
\end{aligned}
$$

The last expression involving consecutive $z_{j}$ 's replaces the three-term recurrence in $v_{j}$ 's. In addition, we need to solve a linear system $M q_{k}=z_{k}$ (7.1) each iteration.
7.1.2. Preconditioned MINRES. From (3.4) and (3.8) we have the following recurrence for the $k$ th column of $D_{k}=V_{k} R_{k}^{-1}$ and $\bar{x}_{k}$ :

$$
d_{k}=\left(v_{k}-\delta_{k}^{(2)} d_{k-1}-\epsilon_{k} d_{k-2}\right) / \gamma_{k}^{(2)}, \quad \bar{x}_{k}=\bar{x}_{k-1}+\tau_{k} d_{k}
$$

Multiplying the above two equations by $M^{-\frac{1}{2}}$ on the left and defining $\bar{d}_{k}=M^{-\frac{1}{2}} d_{k}$, we can update the solution of our original problem by

$$
\bar{d}_{k}=\left(\frac{1}{\beta_{k}} q_{k}-\delta_{k}^{(2)} \bar{d}_{k-1}-\epsilon_{k} \bar{d}_{k-2}\right) / \gamma_{k}^{(2)}, \quad x_{k}=M^{-\frac{1}{2}} \bar{x}_{k}=x_{k-1}+\tau_{k} \bar{d}_{k}
$$

We list the algorithm in [10, Table 3.4].
7.1.3. Preconditioned MINRES-QLP. A preconditioned MINRES-QLP can be derived very similarly. The additional work is to apply right reflectors $P_{k}$ to $R_{k}$, and the new subproblem bases are $W_{k} \equiv V_{k} P_{k}$, with $\bar{x}_{k}=W_{k} u_{k}$. Multiplying the new basis and solution estimate by $M^{-\frac{1}{2}}$ on the left, we obtain

$$
\begin{aligned}
\bar{W}_{k} & \equiv M^{-\frac{1}{2}} W_{k}=M^{-\frac{1}{2}} V_{k} P_{k} \\
x_{k} & =M^{-\frac{1}{2}} \bar{x}_{k}=M^{-\frac{1}{2}} W_{k} u_{k}=\bar{W}_{k} u_{k}=x_{k-2}^{(2)}+\mu_{k-1}^{(2)} \bar{w}_{k-1}^{(3)}+\mu_{k} \bar{w}_{k}^{(2)} .
\end{aligned}
$$

Algorithm 1 lists all steps. Note that $\bar{w}_{k}$ is written as $w_{k}$ for all relevant $k$. Also, the output $x$ solves $A x \approx b$ but the other outputs are associated with $\bar{A} \bar{x} \approx \bar{b}$.

Remark. The requirement of positive-definite preconditioners $M$ in MINRES and MINRES-QLP may seem unnatural for a problem with indefinite $A$ because we cannot achieve $M^{-\frac{1}{2}} A M^{-\frac{1}{2}} \approx I$. However, as shown in [17], we can achieve $M^{-\frac{1}{2}} A M^{-\frac{1}{2}} \approx$ $\left[\begin{array}{ll}I & -I\end{array}\right]$ using an approximate block-LDL ${ }^{\mathrm{T}}$ factorization $A \approx L D L^{T}$ to get $M=$ $L|D| L^{T}$, where $D$ is indefinite with blocks of order 1 and 2 , and $|D|$ has the same eigensystem as $D$ except negative eigenvalues are changed in sign.

SQMR [15] without preconditioning is analytically equivalent to MINRES. Unlike MINRES, SQMR can work directly with an indefinite preconditioner (such as block$L^{\mathrm{T}}$ ). However, in finite precision, SQMR needs "look-ahead" to prevent numerical breakdown.

```
Algorithm 1: Preconditioned MINRES-QLP to solve \((A-\sigma I) x \approx b\).
    input: \(A, b, \sigma, M\)
    \(z_{0}=0, \quad z_{1}=b, \quad\) Solve \(M q_{1}=z_{1}, \quad \beta_{1}=\sqrt{b^{T} q_{1}} \quad\) [Initialize]
    \(w_{0}=w_{-1}=0, \quad x_{-2}=x_{-1}=x_{0}=0\)
    \(c_{0,1}=c_{0,2}=c_{0,3}=-1, \quad s_{0,1}=s_{0,2}=s_{0,3}=0, \quad \phi_{0}=\beta_{1}, \quad \tau_{0}=\omega_{0}=\chi_{-2}=\chi_{-1}=\chi_{0}=0\)
    \(\delta_{1}=\gamma_{-1}=\gamma_{0}=\eta_{-1}=\eta_{0}=\eta_{1}=\vartheta_{-1}=\vartheta_{0}=\vartheta_{1}=\mu_{-1}=\mu_{0}=0, \quad \mathcal{A}=0, \quad \kappa=1\)
    \(k=0\)
    while no stopping condition is satisfied do
        \(k \leftarrow k+1\)
        \(p_{k}=A q_{k}-\sigma q_{k}, \quad \alpha_{k}=\frac{1}{\beta_{k}^{2}} q_{k}^{T} p_{k} \quad\) [Preconditioned Lanczos]
        \(z_{k+1}=\frac{1}{\beta_{k}} p_{k}-\frac{\alpha_{k}}{\beta_{k}} z_{k}-\frac{\beta_{k}}{\beta_{k-1}} z_{k-1}\)
        Solve \(M q_{k+1}=z_{k+1}, \quad \beta_{k+1}=\sqrt{q_{k+1}^{T} z_{k+1}}\)
        if \(k=1\) then \(\rho_{k}=\left\|\left[\begin{array}{ll}\alpha_{k} & \beta_{k+1}\end{array}\right]\right\|\) else \(\rho_{k}=\left\|\left[\begin{array}{lll}\beta_{k} & \alpha_{k} & \beta_{k+1}\end{array}\right]\right\|\)
        \(\delta_{k}^{(2)}=c_{k-1,1} \delta_{k}+s_{k-1,1} \alpha_{k} \quad\) [Previous left reflection...]
        \(\gamma_{k}=s_{k-1,1} \delta_{k}-c_{k-1,1} \alpha_{k} \quad\) [on middle two entries of \(\underline{T_{k}} e_{k} \ldots\) ]
        \(\epsilon_{k+1}=s_{k-1,1} \beta_{k+1} \quad\) [produces first two entries in \(\underline{T_{k+1}} e_{k+1}\) ]
        \(\delta_{k+1}=-c_{k-1,1} \beta_{k+1}\)
        \(c_{k 1}, s_{k 1}, \gamma_{k}^{(2)} \leftarrow \operatorname{SymOrtho}\left(\gamma_{k}, \beta_{k+1}\right) \quad\) [Current left reflection]
        \(c_{k 2}, s_{k 2}, \gamma_{k-2}^{(6)} \leftarrow \operatorname{SymOrtho}\left(\gamma_{k-2}^{(5)}, \epsilon_{k}\right) \quad\) [First right reflection]
        \(\delta_{k}^{(3)}=s_{k 2} \vartheta_{k-1}-c_{k 2} \delta_{k}^{(2)}, \quad \gamma_{k}^{(3)}=-c_{k 2} \gamma_{k}^{(2)}, \quad \eta_{k}=s_{k 2} \gamma_{k}^{(2)}\)
        \(\vartheta_{k-1}^{(2)}=c_{k 2} \vartheta_{k-1}+s_{k 2} \delta_{k}^{(2)}\)
        \(c_{k 3}, s_{k 3}, \gamma_{k-1}^{(5)} \leftarrow \operatorname{SymOrtho}\left(\gamma_{k-1}^{(4)}, \delta_{k}^{(3)}\right) \quad\) [Second right reflection...]
        \(\vartheta_{k}=s_{k 3} \gamma_{k}^{(3)}, \quad \gamma_{k}^{(4)}=-c_{k 3} \gamma_{k}^{(3)} \quad\) [to zero out \(\delta_{k}^{(3)}\) ]
        \(\tau_{k}=c_{k 1} \phi_{k-1} \quad\) [Last element of \(t_{k}\) ]
        \(\phi_{k}=s_{k 1} \phi_{k-1}, \quad \psi_{k-1}=\phi_{k-1}\left\|\left[\begin{array}{ll}\gamma_{k} & \delta_{k+1}\end{array}\right]\right\| \quad\) [Update \(\left.\left\|r_{k}\right\|,\left\|A r_{k-1}\right\|\right]\)
        if \(k=1\) then \(\gamma_{\text {min }}=\gamma_{1}\) else \(\gamma_{\text {min }} \leftarrow \min \left\{\gamma_{\min }, \gamma_{k-2}^{(6)}, \gamma_{k-1}^{(5)},\left|\gamma_{k}^{(4)}\right|\right\}\)
        \(\mathcal{A}^{(k)}=\max \left\{\mathcal{A}^{(k-1)}, \rho_{k}, \gamma_{k-2}^{(6)}, \gamma_{k-1}^{(5)},\left|\gamma_{k}^{(4)}\right|\right\} \quad\) [Update \(\|A\|\) ]
        \(\omega_{k}=\left\|\left[\begin{array}{ll}\omega_{k-1} & \tau_{k}\end{array}\right]\right\|, \quad \kappa \leftarrow \mathcal{A}^{(k)} / \gamma_{\min } \quad\) [Update \(\left.\left\|A x_{k}\right\|, \kappa(A)\right]\)
        \(w_{k}=-\left(c_{k 2} / \beta_{k}\right) q_{k}+s_{k 2} w_{k-2}^{(3)} \quad\) [Update \(\left.w_{k-2}, w_{k-1}, w_{k}\right]\)
        \(w_{k-2}^{(4)}=\left(s_{k 2} / \beta_{k}\right) q_{k}+c_{k 2} w_{k-2}^{(3)}\)
        if \(k>2\) then \(w_{k}^{(2)}=s_{k 3} w_{k-1}^{(2)}-c_{k 3} w_{k}, \quad w_{k-1}^{(3)}=c_{k 3} w_{k-1}^{(2)}+s_{k 3} w_{k}\)
        if \(k>2\) then \(\mu_{k-2}^{(3)}=\left(\tau_{k-2}-\eta_{k-2} \mu_{k-4}^{(4)}-\vartheta_{k-2} \mu_{k-3}^{(3)}\right) / \gamma_{k-2}^{(6)} \quad\) [Update \(\mu_{k-2}\) ]
        if \(k>1\) then \(\mu_{k-1}^{(2)}=\left(\tau_{k-1}-\eta_{k-1} \mu_{k-3}^{(3)}-\vartheta_{k-1}^{(2)} \mu_{k-2}^{(3)}\right) / \gamma_{k-1}^{(5)} \quad\) [Update \(\mu_{k-1}\) ]
        if \(\gamma_{k}^{(4)} \neq 0\) then \(\mu_{k}=\left(\tau_{k}-\eta_{k} \mu_{k-2}^{(3)}-\vartheta_{k} \mu_{k-1}^{(2)}\right) / \gamma_{k}^{(4)}\) else \(\mu_{k}=0 \quad\) [Compute \(\mu_{k}\) ]
        \(x_{k-2}^{(2)}=x_{k-3}^{(2)}+\mu_{k-2}^{(3)} w_{k-2}^{(3)} \quad\) [Update \(\left.x_{k-2}\right]\)
        \(x_{k}=x_{k-2}^{(2)}+\mu_{k-1}^{(2)} w_{k-1}^{(3)}+\mu_{k} w_{k}^{(2)} \quad\) [Compute \(\left.x_{k}\right]\)
        \(\chi_{k-2}^{(2)}=\left\|\left[\chi_{k-3}^{(2)} \mu_{k-2}^{(3)}\right]\right\| \quad \quad\) [Update \(\left.\left\|x_{k-2}\right\|\right]\)
        \(\chi_{k}=\left\|\left[\begin{array}{ccc}\chi_{k-2}^{(2)} & \mu_{k-1}^{(2)} & \mu_{k}\end{array}\right]\right\| \quad\) [Compute \(\left.\left\|x_{k}\right\|\right]\)
    \(x=x_{k}, \quad \phi=\phi_{k}, \quad \psi=\phi_{k}\left\|\left[\begin{array}{ll}\gamma_{k+1} & \delta_{k+2}\end{array}\right]\right\|, \quad \chi=\chi_{k}, \quad \mathcal{A}=\mathcal{A}^{(k)}, \quad \omega=\omega_{k}\)
    output: \(x, \phi, \psi, \chi, \mathcal{A}, \kappa, \omega\)
38
        \(\left[c, s \leftarrow \operatorname{SymOrtho}(a, b)\right.\) is a stable form for computing \(\left.r=\sqrt{a^{2}+b^{2}}, c=\frac{a}{r}, s=\frac{b}{r}\right]\)
```

7.2. Preconditioning singular $A x=b$. For singular compatible systems, MINRES and MINRES-QLP find the minimum-length solution (see Theorems 3.1 and 5.1). If $M$ is nonsingular, the preconditioned system is also compatible and the solvers return its minimum-length solution. The unpreconditioned solution solves $A x \approx b$, but is not necessarily a minimum-length solution.

Example 7.1. Let $A=\left[\begin{array}{llll}1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 & 0\end{array}\right]$ and $b=\left[\begin{array}{l}6 \\ 9 \\ 6 \\ 3\end{array}\right]$. Then $\operatorname{rank}(A)=3$ and $A x=b$ is a singular compatible system. The minimum-length solution is $x^{\dagger}=\left[\begin{array}{lll}2 & 4 & 3\end{array} 2\right]^{T}$. By binormalization [33] we construct the matrix $D=\operatorname{diag}\left(\left[\begin{array}{lll}0.84201 & 0.81228 & 0.30957 \\ 3.2303\end{array}\right]\right)$. The minimum-length solution of the diagonally preconditioned problem $D A D y=D b$ is $y^{\dagger}=[3.57393 .68199 .69090 .93156]^{T}$. Then $x=D y^{\dagger}=\left[\begin{array}{ll}3.0092 & 2.99083 .0000 \\ 3.0092\end{array}\right]^{T}$ is a solution of $A x=b$, but $x \neq x^{\dagger}$.
7.3. Preconditioning singular $A x \approx b$. We propose the following techniques for obtaining minimum-residual solutions of singular incompatible problems. In each case we use an equivalent but larger compatible system to which MINRES may be applied. Even if the larger system is singular, Theorem 3.1 shows that the minimumlength solution of the larger system will be obtained. The required $x$ will be part of this solution. Preconditioning still gives a minimum-residual solution of $A x \approx b$, and in some cases $x$ will be $x^{\dagger}$. If the systems are ill-conditioned, it will be safer and more efficient to apply MINRES-QLP to the original incompatible system. However, preconditioning will give an $x$ that is "minimum length" in a different norm.
7.3.1. Augmented system. When $A$ is singular, so is the augmented system

$$
\left[\begin{array}{ll}
I & A  \tag{7.2}\\
A &
\end{array}\right]\left[\begin{array}{l}
r \\
x
\end{array}\right]=\left[\begin{array}{l}
b \\
0
\end{array}\right],
$$

but it is always compatible. Preconditioning with symmetric positive-definite $M$ gives us a solution $\left[\begin{array}{l}r \\ x\end{array}\right]$ in which $r$ is unique, but $x$ may not be $x^{\dagger}$.
7.3.2. A giant KKT system. Problem (1.1) is equivalent to $\min _{r, x} x^{T} x$ subject to (7.2), which is an equality-contrained convex quadratic program. The corresponding KKT system [36, section 16.1] is both symmetric and compatible:

$$
\left[\begin{array}{cccc} 
& & I & A  \tag{7.3}\\
& -I & A & \\
I & A & & \\
A & & &
\end{array}\right]\left[\begin{array}{l}
r \\
x \\
y \\
z
\end{array}\right]=\left[\begin{array}{l}
0 \\
0 \\
b \\
0
\end{array}\right] .
$$

Although this is still a singular system, the upper-left $3 \times 3$ block-submatrix is nonsingular and therefore $r, x$, and $y$ are unique and a preconditioner applied to the KKT system would give $x$ as the minimum-length solution of our original problem.
7.3.3. Regularization. If the rank of a given matrix $A$ is ill-determined, we may want to solve the regularized problem $[13,22]$ with parameter $\delta>0$ :

$$
\min _{x}\left\|\left[\begin{array}{c}
A  \tag{7.4}\\
\delta I
\end{array}\right] x-\left[\begin{array}{l}
b \\
0
\end{array}\right]\right\|^{2}
$$

The matrix $\left[\begin{array}{c}A \\ \delta I\end{array}\right]$ has full rank and is always better conditioned than $A$. LSQR [40, 41] may be applied, and its iterates $x_{k}$ will reduce $\left\|r_{k}\right\|^{2}+\delta^{2}\left\|x_{k}\right\|^{2}$ monotonically. Alternatively, we could transform (7.4) into the following symmetric compatible systems and apply MINRES or MINRES-QLP. They tend to reduce $\left\|A r_{k}-\delta^{2} x_{k}\right\|$ monotonically.

## Normal equation:

$$
\begin{equation*}
\left(A^{2}+\delta^{2} I\right) x=A b \tag{7.5}
\end{equation*}
$$

## Augmented system:

$$
\left[\begin{array}{cc}
I & A \\
A & -\delta^{2} I
\end{array}\right]\left[\begin{array}{l}
r \\
x
\end{array}\right]=\left[\begin{array}{l}
b \\
0
\end{array}\right]
$$

A two-layered problem: If we eliminate $v$ from the system

$$
\left[\begin{array}{cc}
I & A^{2}  \tag{7.6}\\
A^{2} & -\delta^{2} A^{2}
\end{array}\right]\left[\begin{array}{l}
x \\
v
\end{array}\right]=\left[\begin{array}{c}
0 \\
A b
\end{array}\right]
$$

we obtain (7.5). Thus $x$ is also a solution of our regularized problem (7.4). This is equivalent to the two-layered formulation (4.3) in Bobrovnikova and Vavasis [5] (with $A_{1}=A, A_{2}=D_{1}=D_{2}=I, b_{1}=b, b_{2}=0, \delta_{1}=1$, $\delta_{2}=\delta^{2}$ ). A key property is that $x \rightarrow x^{\dagger}$ as $\delta \rightarrow 0$.
A KKT-like system: If we define $y=-A v$ and $r=b-A x-\delta^{2} y$, then we can show (by eliminating $r$ and $y$ from the following system) that $x$ in

$$
\left[\begin{array}{cccc} 
& & I & A  \tag{7.7}\\
& -I & A & \\
I & A & \delta^{2} I & \\
A & & &
\end{array}\right]\left[\begin{array}{l}
r \\
x \\
y \\
v
\end{array}\right]=\left[\begin{array}{l}
0 \\
0 \\
b \\
0
\end{array}\right]
$$

is also a solution of (7.6) and thus of (7.4). The upper-left $3 \times 3$ blocksubmatrix of (7.7) is nonsingular, and the correct limiting behavior occurs: $x \rightarrow x^{\dagger}$ as $\delta \rightarrow 0$. In fact, (7.7) reduces to (7.3).
7.4. General preconditioners. The construction of preconditioners is usually problem-dependent. If not much is known about the structure of $A$, we can only consider general methods such as diagonal preconditioning and incomplete Cholesky factorization. These methods require access to the nonzero elements of $A$. (They are not applicable if $A$ exists only as an operator for returning the product $A x$.)

For a comprehensive survey of preconditioning techniques, see Benzi [3]. We discuss a few methods for symmetric $A$ that also require access to the nonzero $A_{i j}$.
7.4.1. Diagonal preconditioning. If $A$ has entries that are very different in magnitude, diagonal scaling might improve its condition. When $A$ is diagonally dominant and nonsingular, we can define $D=\operatorname{diag}\left(d_{1}, \ldots, d_{n}\right)$ with $d_{j}=1 /\left|A_{j j}\right|^{1 / 2}$. Instead of solving $A x=b$, we solve $D A D y=D b$, where $D A D$ is still diagonally dominant and nonsingular with all entries $\leq 1$ in magnitude, and $x=D y$.

More generally, if $A$ is not diagonally dominant and possibly singular, we can safeguard division-by-zero errors by choosing a parameter $\delta>0$ and defining

$$
\begin{equation*}
d_{j}(\delta)=1 / \max \left\{\delta, \sqrt{\left|A_{j j}\right|}, \max _{i \neq j}\left|A_{i j}\right|\right\}, \quad j=1, \ldots, n \tag{7.8}
\end{equation*}
$$

Example 7.2.

1. If $A=\left[\begin{array}{cccc}-1 & 10^{-8} & & \\ 10^{-8} & 1 & 10^{4} \\ & 10^{4} & 0 & \\ & & & 0\end{array}\right]$, then $\kappa(A) \approx 10^{4}$. Let $\delta=1, D=\left[\begin{array}{llll}1 & & & \\ & 10^{-2} & & \\ & & 10^{-2} & \\ & & & 1\end{array}\right]$
in (7.8). Then $D A D=\left[\begin{array}{cccc}-1 & 10^{-10} & \\ 10^{-10} & 10^{-4} & 1 \\ & 1 & 0 & \\ & & & 0\end{array}\right]$ and $\kappa(D A D) \approx 1$.
2. $A=\left[\begin{array}{cccc}10^{-4} & 10^{-8} & & \\ 10^{-8} & 10^{-4} & 10^{-8} \\ & 10^{-8} & 0 & \\ & & & 0\end{array}\right]$ contains mostly very small entries, and $\kappa(A) \approx 10^{10}$.

$$
\text { Let } \delta=10^{-8} \text { and } D=\left[\begin{array}{llll}
10^{2} & & & \\
& 10^{2} & & \\
& & 10^{8} & \\
& & & 10^{8}
\end{array}\right] \text {. Then } D A D=\left[\begin{array}{cccc}
1 & 10^{-4} & & \\
10^{-4} & 1 & 10^{2} \\
& 10^{2} & & \\
& & & \\
& & &
\end{array}\right]
$$

and $\kappa(D A D) \approx 10^{2}$. (The choice of $\delta$ makes a critical difference in this case: with $\delta=1$, we have $D=I$.)
7.4.2. Binormalization (BIN). Livne and Golub [33] scale a symmetric matrix by a series of $k$ diagonal matrices on both sides until all rows and columns of the scaled matrix have unit 2-norm: $D A D=D_{k} \cdots D_{1} A D_{1} \cdots D_{k}$. See also Bradley [6].

EXAMPLE 7.3. If $A=\left[\begin{array}{ccc}0^{-8} & 1 & \\ 1 & 10^{-8} & 10^{4} \\ & 10^{4} & 0\end{array}\right]$, then $\kappa(A) \approx 10^{12}$. With just one sweep of BIN, we obtain $D=\operatorname{diag}(8.1 e-3,6.6 e-5,1.5), D A D \approx\left[\begin{array}{ccc}6.5 e-1 & 5.3 e-1 & 0 \\ 5.3 e-1 & 0 & 1 \\ 0 & 1 & 0\end{array}\right]$ and $\kappa(D A D) \approx 2.6$ even though the rows and columns have not converged to one in the two-norm. In contrast, diagonal scaling (7.8) defined by $\delta=1$ and $D=$ $\operatorname{diag}\left(1,10^{-4}, 10^{-4}\right)$ reduces the condition number to approximately $10^{4}$.
7.4.3. Incomplete Cholesky factorization. For a sparse symmetric positive definite matrix $A$, we could compute a preconditioner by the incomplete Cholesky factorization that preserves the sparsity pattern of $A$. This is known as IC0 in the literature. Often there exists a permutation $P$ such that the IC0 factor of $P A P^{T}$ is more sparse than that of $A$.

When $A$ is semidefinite or indefinite, IC0 may not exist, but a simple variant that may work is the incomplete Cholesky-infinity factorization [55, section 5].
8. Numerical experiments. We compare the computed results of MINRESQLP and various other Krylov subspace methods to solutions computed directly by the eigenvalue decomposition (EVD) and the truncated eigenvalue decompositions (TEVD) of $A$. For TEVD we have

$$
x_{t} \equiv \sum_{\left|\lambda_{i}\right|>t\|A\| \varepsilon} \frac{1}{\lambda_{i}} u_{i} u_{i}^{T} b, \quad\|A\|=\max \left|\lambda_{i}\right|, \quad \kappa_{t}(A)=\frac{\max \left|\lambda_{i}\right|}{\min _{\left|\lambda_{i}\right|>t\|A\| \varepsilon}\left|\lambda_{i}\right|}
$$

with parameter $t>0$. Often $t$ is set to 1 , and sometimes to a moderate number such as 10 or 100 ; it defines a cut-off point relative to the largest eigenvalue of $A$. For example, if most eigenvalues are of order 1 in magnitude and the rest are of order $\|A\| \varepsilon \approx 10^{-16}$, we expect TEVD to work better when the small eigenvalues are excluded, while EVD (with $t=0$ ) could return an exploding solution.

In the tables of results, Matlab MinReS and Matlab SYMMLQ are Matlab's implementation of MINRES and SYMMLQ respectively. They incorporate local reorthogonalization of the Lanczos vector $v_{2}$, which could enhance the accuracy of the computations if $b$ is close to an eigenvector of $A$ [32]:

Second Lanczos iteration: $\beta_{1} v_{1}=b$, and $q_{2} \equiv \beta_{2} v_{2}=A v_{1}-\alpha_{1} v_{1}$
Local reorthogonalization: $q_{2} \leftarrow q_{2}-\left(v_{1}^{T} q_{2}\right) v_{1}$.
Lacking the correct stopping condition for singular problems, Matlab SYMMLQ works more than necessary and then selects the smallest residual norm from all computed iterates; it would sometimes report that the method did not converge although the selected estimate appeared to be reasonably accurate.

MINRES SOL and SYMMLQ SOL are implementations based on [39]. MINRES ${ }^{+}$ and SYMMLQ ${ }^{+}$are the same but with additional stopping conditions for singular incompatible systems (see Lemma 3.3 and [10, Proposition 2.12]).

The computations in this section were performed on a Windows XP machine with a 3.2 GHz Intel Pentium D Processor 940 and 3 GB RAM $\left(\varepsilon \approx 10^{-16}\right)$. Tests were performed with each solver on five types of problem:

1. symmetric, nonsingular linear systems
2. symmetric, singular linear systems
3. mildly incompatible symmetric (and singular) systems (meaning $\|r\|$ is rather small with respect to $\|b\|)$
4. symmetric (and singular) LS problems
5. Hermitian systems.

We present a few examples that illustrate the key features of MINRES-QLP. For a larger set of tests and results, such as applying MINRES-QLP and other Krylov methods to Hermitian systems with preconditioning, we refer to [10, Chapter 4].

For a compatible system, we generate a random vector $b$ that is in the range of the test matrix $\left(b \equiv A y, y_{i} \sim i . i . d . U(0,1)\right.$, i.e., $y_{1}, \ldots, y_{n}$ are independent and identically distributed random variables, whose values are drawn from the standard uniform distribution with support $[0,1])$. For an LS problem, we generate a random $b$ that is not in the range of the test matrix $\left(b_{i} \sim i . i . d . U(0,1)\right.$ often suffices $)$.

If $A$ is Hermitian, then $v^{H} A v$ is real for all complex vectors $v$. Numerically (in double precision), $\alpha_{k}=v_{k}^{H} A v_{k}$ is likely to have small imaginary parts in the first few Lanczos iterations and snowball to have large imaginary parts in later iterations. This would result in a poor estimation of $\left\|T_{k}\right\|_{F}$ or $\|A\|_{F}$, and unnecessary errors in the Lanczos vectors. Thus we made sure to typecast $\alpha_{k}=\operatorname{real}\left(v_{k}^{H} A v_{k}\right)$ in MINRES-QLP and MINRES SOL.

We could say from the results that the Lanczos-based methods have built-in regularization features [29], often matching the TEVD solutions very well.
8.1. A Laplacian system $A x \approx b$ (almost compatible). Our first example involves a singular indefinite Laplacian matrix $A$ of order $n=400$. It is blocktridiagonal with each block being a tridiagonal matrix $T$ of order $N=20$ with all nonzeros equal to 1 :

$$
A=\left[\begin{array}{cccc}
T & T & &  \tag{8.1}\\
T & T & \ddots & \\
& \ddots & \ddots & T \\
& & T & T
\end{array}\right]_{n \times n} \quad, \quad T=\left[\begin{array}{cccc}
1 & 1 & & \\
1 & 1 & \ddots & \\
& \ddots & \ddots & 1 \\
& & 1 & 1
\end{array}\right]_{N \times N}
$$

Matlab's eig $(A)$ reports the following data: 205 positive eigenvalues in the interval $[6.1 \mathrm{e}-2,8.87], 39$ almost-zero eigenvalues in $[-2.18 \mathrm{e}-15,3.71 \mathrm{e}-15]$, 156 negative eigenvalues in $[-2.91,-6.65 \mathrm{e}-2]$, numerical rank $=361$.

We used a right-hand side with a small incompatible component: $b=A y+10^{-8} z$ with $y_{i}$ and $z_{i} \sim i . i . d . U(0,1)$. Results are summarized in Table 8.1. In the column labeled "C?", the value "Y" denotes that the associated algorithm in the row has converged to the desired NRBE tolerances within maxit iterations (cf. Table 6.1); otherwise, we have values "N" and "N?", where " N ?" indicates that the algorithm could have converged if more relaxed stopping conditions were used. The column " $A v$ " shows the total number of matrix-vector products, and column " $x(1)$ " lists the

TABLE 8.1
Finite element problem $A x \approx b$ with $b$ almost compatible. Laplacian on a $20 \times 20$ grid, $n=400$, maxit $=1200$, shift $=0$, tol $=1.0 e-15$, maxnorm $=100$, maxcond $=1 e 15,\|b\|=87$. To reproduce this example, run test_minresqlp_eg7_1(24).

| Method | C? | $A v$ | $x(1)$ | $\\|x\\|$ | $\\|e\\|$ | $\\|r\\|$ | $\\|A r\\|$ | $\\|A\\|$ | $\kappa(A)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EVD | - |  | $-7.39 \mathrm{e} 5$ | 4.12 e 7 | 4.1 e 7 | $1.7 \mathrm{e}-7$ | $7.8 \mathrm{e}-7$ | 8.9 e 0 | 1.1 e 17 |
| TEVD | - | - | $3.89 \mathrm{e}-1$ | 1.15 e 1 | 0.0 e 0 | $1.7 \mathrm{e}-8$ | $1.4 \mathrm{e}-12$ | 8.9 e 0 | 1.5 e 2 |
| Matlab SYMMLQ | N? | 371 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $1.4 \mathrm{e}-7$ | $1.8 \mathrm{e}-7$ | $5.8 \mathrm{e}-7$ |  | - |
| SYMMLQ SOL | N | 447 | $-3.08 \mathrm{e} 0$ | 9.63 e 1 | 9.5 e 1 | 1.4 e 2 | 4.4 e 2 | 9.6 e 1 | 1.3 e 1 |
| SYMMLQ ${ }^{+}$ | N | 447 | 2.94 e 6 | 4.27 e 8 | 4.3 e 8 | 1.8 e 2 | 6.5 e 2 | 8.6 e 0 | 1.3 e 1 |
| Matlab MINRES | N | 1200 | $-7.50 \mathrm{e} 5$ | 2.10 e 7 | 2.1 e 7 | 1.5 e 7 | 9.1 e 7 |  |  |
| MINRES SOL | N | 1200 | 9.89 e 5 | 6.10 e 7 | 6.1 e 7 | 2.3 e 7 | 1.5 e 8 | 1.8 e 2 | 1.5 e 1 |
| MINRES ${ }^{+}$ | N | 611 | 1.02 e 0 | 9.28 e 1 | 9.2 e 1 | $1.7 \mathrm{e}-8$ | $2.5 \mathrm{e}-11$ | 8.6 e 0 | 6.9 e 13 |
| MINRES-QLP | Y | 612 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $3.7 \mathrm{e}-11$ | $1.7 \mathrm{e}-8$ | $9.3 \mathrm{e}-11$ | 8.7 e 0 | 4.3 e 13 |
| Matlab LSQR | Y | 1462 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $2.3 \mathrm{e}-13$ | $1.7 \mathrm{e}-8$ | $3.3 \mathrm{e}-13$ |  |  |
| LSQR SOL | Y | 1464 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $2.4 \mathrm{e}-13$ | $1.7 \mathrm{e}-8$ | $3.9 \mathrm{e}-13$ | 1.5 e 2 | 6.4 e 3 |
| Matlab GMRES(30) | N? | 1200 | $3.90 \mathrm{e}-1$ | 1.15 e 1 | $5.2 \mathrm{e}-2$ | $3.4 \mathrm{e}-3$ | $9.4 \mathrm{e}-4$ | - |  |
| SQMR | N | 1200 | $-2.58 \mathrm{e} 8$ | 3.74 e 10 | 3.7 e 10 | 4.6 e 3 | 2.3 e 4 | - |  |
| Matlab QMR | N? | 798 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $5.2 \mathrm{e}-7$ | $1.9 \mathrm{e}-8$ | $2.6 \mathrm{e}-8$ | - | - |
| Matlab BICG | N? | 790 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $4.7 \mathrm{e}-7$ | $3.9 \mathrm{e}-8$ | $1.9 \mathrm{e}-7$ | - | - |
| Matlab BICGSTAB | N? | 2035 | $3.89 \mathrm{e}-1$ | 1.15 e 1 | $4.2 \mathrm{e}-7$ | $1.7 \mathrm{e}-8$ | $4.3 \mathrm{e}-13$ |  | - |

first element of the final solution estimate $x$ for each algorithm. For GMRES, the integer in parentheses is the value of the restart parameter.

MINRES SOL gives a larger solution than MINRES-QLP. This example has a residual norm of about $1.7 \times 10^{-8}$, so it is not clear whether to classify it as a linear system or an LS problem. To the credit of Matlab SYMMLQ, it thinks the system is linear and returns a good solution. For MINRES-QLP, the first 410 iterations are in standard "MINRES mode", with a transfer to "MINRES-QLP mode" for the last 202 iterations. LSQR [40, 41] converges to the minimum-length solution but with more than twice the number of iterations of MINRES-QLP. The other solvers fall short in some way.
8.2. A Laplacian LS problem min $\|A x-b\|$. This example uses the same Laplacian matrix $A$ (8.1) but with a clearly incompatible $b=10 \times \operatorname{rand}(n, 1)$, i.e., $b_{i} \sim i . i . d . U(0,10)$. The residual norm is about 17. Results are summarized in Table 8.2. MINRES gives an LS solution, while MINRES-QLP is the only solver that matches the solution of TEVD. The other solvers do not perform satisfactorily.
8.3. Regularizing effect of MINRES-QLP. This example illustrates the regularizing effect of MINRES-QLP with the stopping condition $\chi_{k} \leq$ maxxnorm. For $k \geq 18$ in Figure 8.1, we observe the following values:

$$
\begin{aligned}
& \chi_{18}=\left\|\left[\begin{array}{lrr}
2.51 & 3.87 \mathrm{e}-11 & 1.38 \times 10^{2}
\end{array}\right]\right\|=1.38 \times 10^{2} \\
& \chi_{19}=\left\|\left[\begin{array}{lrr}
2.51 & -8.00 \mathrm{e}-10 & -1.52 \times 10^{2}
\end{array}\right]\right\|=1.52 \times 10^{2} \\
& \chi_{20}=\left\|\left[\begin{array}{lrr}
2.51 & 1.62 \mathrm{e}-10 & -1.62 \times 10^{6}
\end{array}\right]\right\|=1.62 \times 10^{6}>\text { maxxnorm } \equiv 10^{4} .
\end{aligned}
$$

Because the last value exceeds maxxnorm, MINRES-QLP regards the last diagonal element of $L_{k}$ as a singular value to be ignored (in the spirit of truncated SVD solutions). It discards the last element of $u_{20}$ and updates

$$
\chi_{20} \leftarrow\left\|\left[\begin{array}{lll}
2.51 & 1.62 \mathrm{e}-10 & 0
\end{array}\right]\right\|=2.51
$$

Table 8.2
Finite element problem min $\|A x-b\|$. Laplacian on a $20 \times 20$ grid, $n=400$, maxit $=500$, shift $=0$, tol $=1.0 e-14$, maxnorm $=1 e 4$, maxcond $=1 e 14,\|b\|=120$. To reproduce this example, run test_minresqlp_eg7_1(25).

| Method | $\mathrm{C} ?$ | $A v$ | $x(1)$ | $\\|x\\|$ | $\\|e\\|$ | $\\|r\\|$ | $\\|A r\\|$ | $\\|A\\|$ | $\kappa(A)$ |
| :--- | :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| EVD | - | - | -7.39 e 14 | 4.12 e 16 | 4.1 e 16 | 1.8 e 2 | 7.9 e 2 | 8.9 e 0 | 1.1 e 17 |
| TEVD | - | - | -8.75 e 0 | 1.43 e 2 | 0.0 e 0 | 1.7 e 1 | $4.1 \mathrm{e}-12$ | 8.9 e 0 | 1.5 e 2 |
| MATLAB SYMMLQ | N | 1 | $2.74 \mathrm{e}-1$ | 1.52 e 1 | 1.4 e 2 | 6.0 e 1 | 2.9 e 2 | - | - |
| SYMMLQ SOL | N | 228 | -7.70 e 2 | 9.93 e 3 | 9.9 e 3 | 7.0 e 3 | 3.4 e 4 | 6.8 e 1 | 9.7 e 0 |
| SYMMLQ | N | 228 | -7.70 e 2 | 9.93 e 3 | 9.9 e 3 | 7.0 e 3 | 3.4 e 4 | 7.6 e 0 | 9.7 e 0 |
| MATLAB MINRES | N | 500 | 2.80 e 14 | 4.07 e 16 | 4.1 e 16 | 2.3 e 2 | 1.4 e 3 | - | - |
| MINRES SOL | N | 500 | -1.46 e 14 | 2.11 e 16 | 2.1 e 16 | 1.1 e 2 | 6.6 e 2 | 1.5 e 2 | 1.4 e 1 |
| MINRES + | N | 381 | 3.88 e 1 | 6.90 e 3 | 6.9 e 3 | 1.7 e 1 | $1.2 \mathrm{e}-5$ | 7.9 e 0 | 1.6 e 10 |
| MINRES-QLP | Y | 382 | -8.75 e 0 | 1.43 e 2 | $1.7 \mathrm{e}-6$ | 1.7 e 1 | $1.7 \mathrm{e}-5$ | 8.6 e 0 | 3.5 e 10 |
| MATLAB LSQR | Y | 1000 | -8.75 e 0 | 1.43 e 2 | $2.0 \mathrm{e}-5$ | 1.7 e 1 | $1.4 \mathrm{e}-5$ | - | - |
| LSQR SOL | Y | 1000 | -8.75 e 0 | 1.43 e 2 | $2.3 \mathrm{e}-5$ | 1.7 e 1 | $1.1 \mathrm{e}-5$ | 1.2 e 2 | 4.4 e 3 |
| MATLAB GMRES(30) | N | 500 | -8.84 e 0 | 1.25 e 2 | 4.8 e 1 | 1.7 e 1 | $8.2 \mathrm{e}-1$ | - | - |
| SQMR | N | 500 | 9.58 e 15 | 1.39 e 18 | 1.4 e 18 | 1.2 e 11 | 6.7 e 11 | - | - |
| MATLAB QMR | N | 556 | -7.30 e 0 | 1.92 e 2 | 1.4 e 2 | 1.7 e 1 | 1.2 e 1 | - | - |
| MATLAB BICG | N | 2 | 1.40 e 0 | 1.71 e 1 | 1.4 e 2 | 6.0 e 1 | 2.6 e 2 | - | - |
| MATLAB BICGSTAB | N | 104 | -1.12 e 1 | 1.40 e 2 | 9.6 e 1 | 2.6 e 1 | 1.8 e 1 | -- | -- |

The full truncation strategy used in the implementation is justified by the fact that $x_{k}=W_{k} u_{k}$ with $W_{k}$ orthogonal. When $\left\|x_{k}\right\|$ becomes large, the last element of $u_{k}$ is treated as zero. If $\left\|x_{k}\right\|$ is still large, the second-to-last element of $u_{k}$ is treated as zero. If $\left\|x_{k}\right\|$ is still large, the third-to-last element of $u_{k}$ is treated as zero.
8.4. Effects of rounding errors in MINRES-QLP. The recurred residual norms $\phi_{k}^{M}$ in MINRES usually approximate the directly computed ones $\left\|r_{k}^{M}\right\|$ very well until $\left\|r_{k}^{M}\right\|$ becomes small. We observe that $\phi_{k}^{M}$ continues to decrease in the last few iterations, even though $\left\|r_{k}^{M}\right\|$ has become stagnant. This is desirable in the sense that the stopping rule will cause termination, although the final solution is not as accurate as predicted.

We present similar plots of MINRES-QLP in the following examples, with the corresponding quantities as $\phi_{k}^{Q}$ and $\left\|r_{k}^{Q}\right\|$. We observe that except in very ill-conditioned LS problems, $\phi_{k}^{Q}$ approximates $\left\|r_{k}^{Q}\right\|$ very closely.

Figure 8.2 illustrates four singular compatible linear systems.
Figure 8.3 illustrates four singular LS problems.
9. Conclusion. MINRES constructs its $k$ th solution estimate from the recursion $x_{k}=D_{k} t_{k}=x_{k-1}+\tau_{k} d_{k}(3.4)$, where $n$ separate triangular systems $R_{k}^{T} D_{k}^{T}=V_{k}^{T}$ are solved to obtain the $n$ elements of each direction $d_{1}, \ldots, d_{k}$. (Only $d_{k}$ is obtained during iteration $k$, but it has $n$ elements.)

In contrast, MINRES-QLP constructs its $k$ th solution estimate using orthogonal steps: $x_{k}^{Q}=\left(V_{k} P_{k}\right) u_{k}$; see (5.3)-(5.9). Only one triangular system $L_{k} u_{k}=Q_{k}\left(\beta_{1} e_{1}\right)$ is involved for each $k$.

Thus MINRES-QLP overcomes the potential instability predicted by the MINRES authors [39] and analyzed by Sleijpen et al. [47]. The additional work and storage are moderate, and maximum efficiency is retained by transferring from MINRES to the MINRES-QLP iterates only when the estimated condition number of $A$ exceeds a specified value.


FIG. 8.1. Recurred $\phi_{k} \approx\left\|r_{k}\right\|, \psi_{k} \approx\left\|A r_{k}\right\|$, and $\left\|x_{k}\right\|$ for MINRES and MINRES-QLP. The matrix A (ID 1177 from [54]) is positive semidefinite, $n=25$, and $b$ is random with $\|b\| \simeq 1.7$. $B$ oth solvers could have achieved essentially the TEVD solution of $A x \simeq b$ at iteration 11. However, the stringent tol $=10^{-14}$ on the recurred normwise relative backward errors (NRBE in Table 6.1) prevents them from stopping "in time". MINRES ends with an exploding solution, yet MINRES$Q L P$ brings it back to the TEVD solution at iteration 20. Left: $\phi_{k}^{M}$ and $\phi_{k}^{Q}$ (recurred $\left\|r_{k}\right\|$ of MINRES and MINRES-QLP) and their NRBE. Middle: $\psi_{k}^{M}$ and $\psi_{k}^{Q}$ (recurred $\left\|A r_{k}\right\|$ ) and their NRBE. Right: $\left\|x_{k}^{M}\right\|$ (norms of solution estimates from MINRES) and $\chi_{k}^{Q}$ (recurred $\left\|x_{k}\right\|$ from MINRES-QLP) with maxxnorm $=10^{4}$. This figure can be reproduced by test_minresqlp_fig7_1 (2).

MINRES and MINRES-QLP are readily applicable to Hermitian matrices, once $\alpha_{k}$ is typecast as a real scalar in finite-precision arithmetic. For both algorithms, we derived recurrence relations for $\left\|A r_{k}\right\|$ and $\left\|A x_{k}\right\|$ and used them to formulate new stopping conditions for singular problems.

TEVD or TSVD are commonly known to use rank- $k$ approximations to $A$ to find approximate solutions to min $\|A x-b\|$ that serve as a form of regularization. Krylov subspace methods also have regularization properties [23, 21, 29]. Since MINRESQLP monitors more carefully the rank of $T_{k}$, which could be $k$ or $k-1$, we may say that regularization is a stronger feature in MINRES-QLP, as we have shown in our numerical examples.

It is important to develop robust techniques for estimating an a priori bound for the solution norm since the MINRES-QLP approximations are not monotonic as is the case in CG and LSQR. Ideally, we would also like to determine a practical threshold associated with the stopping condition $\gamma_{k}^{(4)}=0$ in order to handle cases when $\gamma_{k}^{(4)}$ is numerically small but not exactly zero. These are topics for future research.
10. Software and reproducible research. MATLAB 7.6, Fortran 77, and Fortran 90 implementations of MINRES with new stopping conditions $\left\|A r_{k}\right\| \leq t o l\|A\|\left\|r_{k}\right\|$ and $\left\|A x_{k}\right\| \leq t o l\|A\|\left\|x_{k}\right\|$, and a MATLAB 7.6 implementation of MINRES-QLP are available from SOL [48].

Following the philosophy of reproducible computational research as advocated in $[11,9]$, for each figure and example in this paper we mention either the source or the specific Matlab command. Our Matlab scripts are available at SOL [48].


Fig. 8.2. Solving $A x=b$ with semidefinite $A$ similar to an example of Sleijpen et al. [47]. $A=Q \operatorname{diag}\left(\left[0_{5}, \eta, 2 \eta, 2: \frac{1}{789}: 3\right]\right) Q$ of dimension $n=797$, nullity 5 , and norm $\|A\|=3$, where $Q=I-(2 / n) w w^{T}$ is a Householder matrix generated by $v=\left[0_{5}, 1, \ldots, 1\right]^{T}, w=v /\|v\|$. These plots illustrate and compare the effect of rounding errors in MINRES and MINRES-QLP.

The upper part of each plot shows the computed and recurred residual norms, and the lower part shows the computed and recurred normwise relative backward errors (NRBE, defined in Table 6.1). MINRES and MINRES-QLP terminate when the recurred NRBE is less than the given tol $=10^{-14}$.

Upper left: $\eta=10^{-8}$ and thus $\kappa(A) \approx 10^{8}$. Also $b=e$ and therefore $\|x\| \gg\|b\|$. The graphs of MINRES's directly computed residual norms $\left\|r_{k}^{M}\right\|$ and recurrently computed residual norms $\phi_{k}^{M}$ start to differ at the level of $10^{-1}$ starting at iteration 21, while the values $\phi_{k}^{Q} \approx\left\|r_{k}^{Q}\right\|$ from MINRES-QLP decrease monotonically and stop near $10^{-6}$ at iteration 26.

Upper right: Again $\eta=10^{-8}$ but $b=$ Ae. Thus $\|x\|=\|e\|=O(\|b\|)$. The MINRES graphs of $\left\|r_{k}^{M}\right\|$ and $\phi_{k}^{M}$ start to differ when they reach a much smaller level of $10^{-10}$ at iteration 30. The MINRES-QLP $\phi_{k}^{Q}$ 's are excellent approximations of $\phi_{k}^{Q}$, with both reaching $10^{-13}$ at iteration 33.

Lower left: $\eta=10^{-10}$ and thus $A$ is even more ill-conditioned than the matrix in the upper plots. Here $b=e$ and $\|x\|$ is again exploding. MINRES ends with $\left\|r_{k}^{M}\right\| \approx 10^{2}$, which means no convergence, while MINRES-QLP reaches a residual norm of $10^{-4}$.

Lower right: $\eta=10^{-10}$ and $b=$ Ae. The final MINRES residual norm $\left\|r_{k}^{M}\right\| \approx 10^{-8}$, which is satisfactory but not as accurate as $\phi_{k}^{M}$ claims at $10^{-13}$. MINRES-QLP again has $\phi_{k}^{Q} \approx\left\|r_{k}^{Q}\right\| \approx$ $10^{-13}$ at iteration 37.

This figure can be reproduced by DPtestSing7.m.


Fig. 8.3. Solving $A x=b$ with semidefinite $A$ similar to an example of Sleijpen et al. [47]. $A=Q \operatorname{diag}\left(\left[0_{5}, \eta, 2 \eta, 2: \frac{1}{789}: 3\right]\right) Q$ of dimension $n=797$ with $\|A\|=3$, where $Q=I-(2 / n) e e^{T}$ is a Householder matrix generated by $e=[1, \ldots, 1]^{T}$. (We are not plotting the NRBE quantities because $\|A\|\left\|r_{k}\right\| \approx 6$ throughout the iterations in this example.)

Upper left: $\eta=10^{-2}$ and thus $\operatorname{cond}(A) \approx 10^{2}$. Also $b=e$ and therefore $\|x\| \gg\|b\|$. The graphs of MINRES's directly computed $\left\|A r_{k}^{M}\right\|$ and recurrently computed $\psi_{k}^{M}$, and also $\psi_{k}^{Q} \approx\left\|A r_{k}^{Q}\right\|$ from MINRES-QLP, match very well throughout the iterations.

Upper right: Here, $\eta=10^{-4}$ and $A$ is more ill-conditioned than the last example (upper left). The final MINRES residual norm $\psi_{k}^{M} \approx\left\|A r_{k}^{M}\right\|$ is slightly larger than the final MINRES-QLP residual norm $\psi_{k}^{Q} \approx\left\|A r_{k}^{Q}\right\|$. The MINRES-QLP $\psi_{k}^{Q}$ are excellent approximations of $\left\|A r_{k}^{Q}\right\|$.

Lower left: $\eta=10^{-6}$ and $\operatorname{cond}(A) \approx 10^{6}$. MINRES's $\psi_{k}^{M}$ and $\left\|A r_{k}^{M}\right\|$ differ starting at iteration 21. Eventually, $\left\|A r_{k}^{M}\right\| \approx 3$, which means no convergence. MINRES-QLP reaches a residual norm of $\psi_{k}^{Q}=\left\|A r_{k}^{Q}\right\|=10^{-2}$.

Lower right: $\eta=10^{-8}$. MINRES performs even worse than in the last example (lower left). MINRES-QLP reaches a minimum $\left\|A r_{k}^{Q}\right\| \approx 10^{-7}$ but tol $=10^{-8}$ does not shut it down soon enough. The final $\psi_{k}^{Q}=\left\|A r_{k}^{Q}\right\|=10^{-2}$. The values of $\psi_{k}^{Q}$ and $\left\|A r_{k}^{Q}\right\|$ differ only at iterations 27-28.

This figure can be reproduced by DPtestLSSing5.m.

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Appendix A. Proof that $T_{\ell}$ is nonsingular iff $b \in \operatorname{range}(A)$ (section 2.1).
If $T_{\ell}$ is nonsingular, we have $A V_{\ell} T_{\ell}^{-1} e_{1}=V_{\ell} e_{1}=\beta_{1}^{-1} b$. Conversely, if $b \in$ $\operatorname{range}(A)$, then $\operatorname{range}\left(V_{\ell}\right) \subseteq \operatorname{range}(A)$ and $\operatorname{null}(A) \cap \operatorname{range}\left(V_{\ell}\right)=\{0\}$. We also know that $\operatorname{rank}\left(V_{\ell}\right)=\ell \operatorname{and} \operatorname{rank}\left(T_{\ell}\right)=\operatorname{rank}\left(V_{\ell} T_{\ell}\right)=\operatorname{rank}\left(A V_{\ell}\right)=\operatorname{rank}\left(V_{\ell}\right)-\operatorname{dim}[\operatorname{null}(A) \cap$ $\left.\operatorname{range}\left(V_{\ell}\right)\right]$; see [4, Fact 2.10.4 ii]. Thus $\operatorname{rank}\left(T_{\ell}\right)=\ell$ and so $T_{\ell}$ is nonsingular.)

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[^1]:    ${ }^{1}$ Numerically, $p_{k}=A v_{k}-\beta_{k} v_{k-1}, \alpha_{k}=v_{k}^{T} p_{k}, \beta_{k+1} v_{k+1}=p_{k}-\alpha_{k} v_{k}$ is slightly better [38].

