TriCG AND TriMR: TWO ITERATIVE METHODS FOR SYMMETRIC QUASI-DEFINITE SYSTEMS

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Abstract. We introduce iterative methods named TriCG and TriMR for solving symmetric quasi-definite systems based on the orthogonal tridiagonalization process proposed by Saunders, Simon and Yip in 1988. TriCG and TriMR are tantamount to preconditioned Block-Cg and Block-Minres with two right-hand sides in which the two approximate solutions are summed at each iteration, but require less storage and work per iteration. We evaluate the performance of TriCG and TriMR on linear systems generated from the SuiteSparse Matrix Collection and from discretized and stabilized Stokes equations. We compare TriCG and TriMR with Symmlq and Minres, the recommended Krylov methods for symmetric and indefinite systems. In all our experiments, TriCG and TriMR terminate earlier than Symmlq and Minres on a residual-based stopping condition with an improvement of up to 50% in terms of number of iterations. They also terminate more reliably than Block-Cg and Block-Minres. Experiments in quadruple and octuple precision suggest that loss of orthogonality in the basis vectors is significantly less pronounced in TriCG and TriMR than in Block-Cg and Block-Minres.

Key words. iterative methods, orthogonal tridiagonalization process, block-Lanczos process, Krylov subspaces, symmetric quasi-definite systems, saddle-point systems, interior-point methods, stabilized Stokes equations

AMS subject classifications. 15A06, 65F10, 65F08, 65F22, 65F25, 65F50, 90C06, 90C90

1. Introduction. Consider a linear system of the form

\[
\begin{bmatrix}
M & A \\
A^T & -N
\end{bmatrix}
\begin{bmatrix}
x \\
y
\end{bmatrix}
=
\begin{bmatrix}
b \\
c
\end{bmatrix},
\]

where \( M \in \mathbb{R}^{m \times m} \) and \( N \in \mathbb{R}^{n \times n} \) are symmetric positive definite, \( b \in \mathbb{R}^m \) and \( c \in \mathbb{R}^n \) are not simultaneously zero, and \( A \in \mathbb{R}^{m \times n} \) can have any shape.

We use the definition given by Orban and Arioli (2017): a matrix \( K \) is symmetric quasi-definite (SQD) if \( K = K^T \) and there exists a permutation matrix \( P \) such that \( P^T K P \) has the form (1.1). In particular, (1.1) arises in interior-point methods for inequality-constrained optimization (Altmann and Gondzio, 1999; Friedlander and Orban, 2012) and in the context of stabilized mixed finite elements methods (Elman, Silvester, and Wathen, 2014). SQD matrices are indefinite and nonsingular (Vanderbei, 1995).

In this paper, we develop two iterative methods named TriCG and TriMR specialized for (1.1), based on the orthogonal tridiagonalization process in elliptic norms and a closely-related formulation as a preconditioned block-Lanczos method. Relations between both processes are described in detail and we show how the preconditioned block-Lanczos process with two specific right-hand sides can generate structured Krylov bases with SQD systems. Our main motivation for developing TriCG and TriMR comes from an absence of iterative methods for (1.1) that exploit the SQD structure when both \( b \) and \( c \) are nonzero.

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The rest of this paper is organized as follows. We state the defining properties of TriCG of TriMR and describe their implementations in detail. In a second stage, we compare TriCG and TriMR with their block counterparts Block-Cg and Block-Minres as well as Symmlq and Minres on two set of problems. The first set uses the SuiteSparse Matrix Collection without preconditioning. The second set is composed of discretized and stabilized Stokes equations and requires preconditioning. Finally, we discuss extensions of TriCG and TriMR and their uses outside the context of SQD systems.

Related research. Orban and Arioli (2017) expose the state of the art on iterative methods for SQD systems. They explain that existing Krylov methods for symmetric indefinite systems, such as Symmlq and Minres (Paige and Saunders, 1975) or Minres-qlp (Choi, Paige, and Saunders, 2011) do not exploit the rich structure of (1.1). Cg (Hestenes and Stiefel, 1952) is well defined on (1.1) provided \( b = 0 \) or \( c = 0 \). Otherwise, it may break down. For example, any SQD system such that \( b^T Mb + 2b^T Ac - c^T Nc = 0 \) causes breakdown on the first Cg iteration. Orban and Arioli (2017) show that preconditioned and regularized Lsqr (Paige and Saunders, 1982) and Lsmr (Fong and Saunders, 2011) take advantage of block structure to solve (1.2)

\[
\begin{bmatrix}
M \\ A^T - N
\end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix},
\]

and are equivalent to Cg and Minres applied to the normal equations

\[
(A^T M^{-1} A + N)y = A^T M^{-1} b \quad \text{with} \quad x = M^{-1} (b - Ay).
\]

They also show that preconditioned and regularized CRAIG (Craig, 1955) and CRAIGMR (Orban and Arioli, 2017) solve

\[
\begin{bmatrix}
M \\ A^T - N
\end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ c \end{bmatrix},
\]

and are equivalent to Cg and Minres applied to the Schur-complement equations

\[
(A^T M^{-1} A + N)y = -c \quad \text{with} \quad x = -M^{-1} Ay.
\]

In a similar vein, Estrin, Orban, and Saunders (2019a,b) develop LSLQ and LNLQ to solve (1.2) and (1.4), respectively; and explain that preconditioned and regularized variants of those methods are equivalent to Symmlq applied to (1.3) and to (1.5).

When \( b \neq 0 \) and \( c \neq 0 \), one possibility is to shift the right-hand side to recover (1.2) or (1.4). For instance, we can solve \(-N\Delta y = c\) and add \((0, \Delta y)\) to the solution of (1.2) with right-hand side \((b - A\Delta y, 0)\). Buttari, Orban, Ruiz, and Titley-Peloquin (2019) developed USYMLQR upon the orthogonal tridiagonalization process (Saunders, Simon, and Yip, 1988), henceforth the SSY process, for the saddle-point system

\[
\begin{bmatrix}
M \\ A^T \\ 0
\end{bmatrix} \begin{bmatrix} x \\ y \\ 0 \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}.
\]

The SSY process requires two initial vectors, which makes it ideal to develop TriCG and TriMR, two methods specialized for SQD systems in the case where both \( b \) and \( c \) are nonzero. Its close relation to a block-Lanczos process induces similarities between TriCG and the block-Cg method (O’Leary, 1980) as well as...
TriMR and block-MINRES methods. The block-Lanczos process was initially developed to compute eigenvalues (Golub and Underwood, 1977). Thereafter it was used to find nullspaces (Montgomery, 1995) and solve linear systems with multiple right-hand sides (Guennouni, Jbilou, and Sadok, 2004). In this paper, a novel application of this process is presented for SQD linear systems with a single right-hand side.

**Notation.** Vectors and scalars are denoted by lowercase Latin and Greek letters, respectively. Matrices are denoted by capital Latin letters, except for $2 \times 2$ blocks, which are represented by capital Greek letters. Rare exceptions to those rules are indicated explicitly in the text. For a vector $v$, $\|v\|$ denotes the Euclidean norm of $v$, and for a symmetric and positive-definite matrix $M$, the $M$-norm of $v$ is $\|v\|_M^2 = v^TMv$. The shorthand $v \mapsto M \setminus v$ represents an operator that returns the solution of $M u = v$. The vector $e_i$ is the $i$-th column of an identity matrix of size dictated by the context. $I_k$ represents the $k \times k$ identity operator. The shorthand $\text{diag}(\omega_1, \ldots, \omega_k)$ represents the $k \times k$ diagonal matrix with $\omega_1, \ldots, \omega_k$ on its diagonal. We denote by $K$ the SQD matrix of (1.1) and

\[
(1.7) \quad K_0 := \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}, \quad H := \text{blkdiag}(M, N) = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix}, \quad B := \begin{bmatrix} b & 0 \\ 0 & c \end{bmatrix}.
\]

We abuse notation and write $(b, c)$ to represent the column vector $[b^T \ c^T]^T$.

2. **Processes.** In this section, we state the SSY process in elliptic norms, which is the foundation for the development of the methods TriCG and TriMR, its relation with the preconditioned block-Lanczos process, and how they can accommodate regularization.

2.1. **The orthogonal tridiagonalization process in elliptic norms.** The SSY process generalized by Buttari et al. (2019) in terms of elliptic norms defined by positive definite $M$ and $N$ generates sequences of vectors $v_k$ and $u_k$ such that $v_i^T M v_j = \delta_{ij}$ and $u_i^T N u_j = \delta_{ij}$ in exact arithmetic. The process is stated as Algorithm 2.1, where we use the shorthand notation $\beta_1 M v_1 = b$ to summarize the normalization operations

1. set $\bar{v}_1 = b$;
2. solve $M v_1 = \bar{v}_1$;
3. compute $\beta_1 = (\bar{v}_1^T v_1)^{\frac{1}{2}}$;
4. normalize $\bar{v}_1 \leftarrow \bar{v}_1 / \beta_1$ and $v_1 \leftarrow v_1 / \beta_1$,

and similarly for $\gamma_1 N u_1 = c$ and subsequent normalization steps. When $M$ and $N$ are not the identity, the above normalization operations only require solves with $M$ and $N$. Occurrences of $M v_k$ and $N u_k$ in a right-hand side in Algorithm 2.1 simply mean that we substitute $\bar{v}_k$ and $\bar{u}_k$, respectively, so that $M$ and $N$ themselves are not needed. The process terminates if there exists an index $k$ such that $\beta_{k+1} = 0$ or $\gamma_{k+1} = 0$.

We denote $V_k = [v_1 \ldots v_k]$ and $U_k = [u_1 \ldots u_k]$. After $k$ iterations of Algorithm 2.1, the situation may be summarized as

\[
(2.1a) \quad A U_k = M V_k T_k + \beta_{k+1} M v_{k+1} e_k^T = M V_{k+1} T_{k+1,k} \\
(2.1b) \quad A^T V_k = N U_k T_k + \gamma_{k+1} N u_{k+1} e_k = N U_{k+1} T_{k,k+1} \\
(2.1c) \quad V_k^T M V_k = U_k^T N U_k = I_k,
\]
**Algorithm 2.1** Orthogonal Tridiagonalization Process in Elliptic Norms

**Require:** $A$, $b$, $c$, $v \mapsto Mv$, $u \mapsto Nu$

1. $v_0 = 0$, $u_0 = 0$
2. $\beta_1 M v_1 = b$, $\gamma_1 N u_1 = c$ (so that $||v_1||_M = ||u_1||_N = 1$
3. for $k = 1, 2, \ldots$ do
4. \hspace{1em} $q = Au_k - \gamma_k M v_{k-1}$, $\alpha_k = v_k^T q$
5. \hspace{1em} $p = A^T v_k - \beta_k N u_{k-1}$
6. \hspace{1em} $\beta_{k+1} M v_{k+1} = q - \alpha_k M v_k$ $\beta_{k+1} > 0$ so that $||v_{k+1}||_M = 1$
7. \hspace{1em} $\gamma_{k+1} N u_{k+1} = p - \alpha_k N u_k$ $\gamma_{k+1} > 0$ so that $||u_{k+1}||_N = 1$
8. end for

where

$$T_k = \begin{bmatrix} \alpha_1 & \gamma_2 \\ \beta_2 & \alpha_2 & \ddots \\ \vdots & \ddots & \ddots & \gamma_k \\ \beta_k & \alpha_k \end{bmatrix}, \quad T_{k,k+1} = \begin{bmatrix} T_k & \gamma_{k+1} e_k \end{bmatrix}, \quad T_{k+1,k} = \begin{bmatrix} T_k^T \beta_{k+1} e_k^T \end{bmatrix}.$$

Equations (2.1a)-(2.1b) hold to within machine precision despite loss of orthogonality, but (2.1c) and $V_k^T A U_k = T_k$ hold only in exact arithmetic.

### 2.2. Relation with preconditioned block-Lanczos process

Saunders et al. (1988) note Beresford Parlett’s observation that the subspaces generated by Algorithm 2.1 in the Euclidean norm can be viewed as the union of those generated by the block-Lanczos process applied to $AA^T$ and $A^T A$ with respective starting blocks $[c \ A^T b]$ and $[b \ A c]$. Golub, Stoll, and Wathen (2008) pushed the observation further in terms of the block-Lanczos process applied to $K_0$ in (1.7). This section summarizes the latter observations and incorporates the preconditioner $H$.

Pasting (2.1) together results in

$$\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} V_k & 0 \\ 0 & U_k \end{bmatrix} = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix} \begin{bmatrix} V_{k+1} & 0 \\ 0 & U_{k+1} \end{bmatrix} \begin{bmatrix} 0 & T_{k+1,k} \\ T_{k,k+1}^T & 0 \end{bmatrix},$$

which resembles a Krylov process in which basis vectors have been permuted. Let

$$P_k := \begin{bmatrix} e_1 & e_{k+1} & \cdots & e_i & e_{k+i} & \cdots & e_k & e_{2k} \end{bmatrix} = [E_1 \cdots E_k] \quad \text{where} \quad E_k = \begin{bmatrix} e_k & e_k \end{bmatrix},$$

denote the permutation, introduced by Paige (1974), that restores the order in which Algorithm 2.1 generates basis vectors:

$$W_k := \begin{bmatrix} V_k & 0 \\ 0 & U_k \end{bmatrix} P_k = [w_1 \cdots w_k] \quad \text{where} \quad w_k = \begin{bmatrix} v_k & 0 \\ 0 & u_k \end{bmatrix}.$$

Although $w_k$ is a matrix, we use a lowercase letter due to the close link with the vectors $v_k$ and $u_k$. The projection of $K_0$ in the Krylov subspace $\text{Span}\{v_1, \ldots, w_k\}$ is also shuffled to symmetric block-tridiagonal form with blocks of size 2:

$$K_0 W_k = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix} \begin{bmatrix} V_{k+1} & 0 \\ 0 & U_{k+1} \end{bmatrix} P_{k+1} P_k^T \begin{bmatrix} 0 & T_{k+1,k} \\ T_{k,k+1}^T & 0 \end{bmatrix}.$$

$$= HW_{k+1} F_{k+1,k},$$
where
\[
F_{k+1,k} = \begin{bmatrix}
\Omega_1 & \Psi_2 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\Psi_2^T & \Omega_2 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\Psi_k^T & \Omega_k & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\Omega_k & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\Psi_{k+1}^T & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{bmatrix}
\]
\[
\Omega_k = \begin{bmatrix} 0 & \alpha_k \\ \alpha_k & 0 \end{bmatrix}, \quad \Psi_k = \begin{bmatrix} 0 & \gamma_k \\ \beta_k & 0 \end{bmatrix}.
\]

The two relations at line 2 of Algorithm 2.1 can be rearranged as
\[(2.5) \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix} \begin{bmatrix} v_1 & 0 \\ 0 & u_1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ 0 \end{bmatrix} = \begin{bmatrix} b & 0 \\ 0 & c \end{bmatrix} \iff Hw_1\Psi_1^T = B.\]

The identities (2.4) and (2.5) characterize the preconditioned block-Lanczos process applied to $K_0$ with preconditioner $H$ and initial block $B$. We summarize the process as Algorithm 2.2 where all $w_k \in \mathbb{R}^{(n+m)\times 2}$ and $\Psi_k \in \mathbb{R}^{2\times 2}$ are determined such that both $w_k^T H w_k = I_2$ and the equations on lines 2 and 5 are verified.

**Algorithm 2.2 Preconditioned Block-Lanczos Process**

**Require:** $K_0$, $B$, $w \mapsto Hw$

1: $w_0 = 0$
2: $Hw_1\Psi_1^T = B$
3: for $k = 1, 2, \ldots$ do
4: $\Omega_k = w_k^T K_0 w_k$
5: $Hw_{k+1}\Psi_{k+1} = K_0 w_k - Hw_k \Omega_k - Hw_{k-1} \Psi_k$
6: end for

Note that Algorithm 2.1 and Algorithm 2.2 require operators that return the solution of systems with coefficient $M$, $N$ and $H$. A specificity of Algorithm 2.2 is that $w_k$ and $\Psi_k$ are not unique. They are commonly determined from the Gram-Schmidt process: $w_k \Psi_k^T$ is the QR decomposition of the right-hand side on lines 2 and 5 of Algorithm 2.2. For instance, $F_{k+1,k}$ is pentadiagonal when we force $\Psi_k = \text{diag}(\beta_k, \gamma_k)$ for all $k$, in which case the structure of $w_k$ is
\[
w_k = \begin{bmatrix} v_k & 0 \\ 0 & u_k \end{bmatrix} \quad (k \text{ odd}) \quad \text{and} \quad w_k = \begin{bmatrix} 0 & v_k \\ u_k & 0 \end{bmatrix} \quad (k \text{ even}).
\]

### 2.3. Regularization of the preconditioned block-Lanczos process.

**Theorem 2.1.** Given the SQD matrix $K$ and block right-hand side $B$, the preconditioned Krylov basis $W_k$ generated by Algorithm 2.2 has the form (2.3) where the vectors $u_k$ and $v_k$ are the same as those generated by Algorithm 2.1 with initial vectors $b$ and $c$. In addition,

\[(2.6) \quad KW_k = HW_{k+1}S_{k+1,k}, \quad S_{k+1,k} := \begin{bmatrix} \Theta_1 & \Psi_2 & \cdots & \cdots & \cdots \\ \Psi_2^T & \Theta_2 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \Theta_k & \cdots & \cdots & \cdots & \cdots \\ \Psi_k^T & \cdots & \cdots & \cdots & \cdots \\ \Psi_{k+1}^T & \cdots & \cdots & \cdots & \cdots \end{bmatrix}.
\]
where
\[ \Theta_k = \begin{bmatrix} 1 & \alpha_k \\ \alpha_k & -1 \end{bmatrix} \quad \text{and} \quad \Psi_k = \begin{bmatrix} 0 & \gamma_k \\ \beta_k & 0 \end{bmatrix}. \]
The scalars \( \alpha_k, \beta_k \) and \( \gamma_k \) are those generated by Algorithm 2.1 when it is applied to \( A \) with initial vectors \( b \) and \( c \).

**Proof.** Observe that \( K = K_0 + \text{blkdiag}(M, -N) \). Algorithm 2.2 applied to \( K_0 \) generates sparse pairs \( w_k \) as in (2.3) because of the equivalence with Algorithm 2.1. The term \( \text{blkdiag}(M, -N) \) can be seen as a regularization term:

\[ \left( \begin{array}{cc} M & 0 \\ 0 & -N \end{array} \right) w_k = H w_k \Lambda_k \quad \text{with} \quad \Lambda_k := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \]
The identities (2.4) and (2.7) allow us to write

\[ (2.8) \quad KW_k = H \begin{pmatrix} \Omega_1 + \Lambda_1 & \Psi_2 \\ \Psi_2^T & \cdots & \Psi_k^T \\ \cdots & \cdots & \Psi_k^T \\ \Psi_k & \Omega_k + \Lambda_k \end{pmatrix} + w_{k+1} \Psi_k^T, \]

which amounts to (2.6) because \( \Theta_k = \Omega_k + \Lambda_k \). The Krylov basis \( W_k \) is not modified; only the projection of \( K \) in the Krylov subspace is updated.

Because of Theorem 2.1, the Krylov basis \( W_k \) generated by Algorithm 2.2 must have the sparsity structure (2.3), so that only \( u_k \) and \( v_k \) need be generated, and they may be generated directly from Algorithm 2.1. In addition, products with \( M \) and \( N \) are not required to generate \( W_k \), so that the computational cost per iteration is reduced and less storage is required compared to Algorithm 2.2.

**3. Methods.** In this section, we develop two methods based upon Algorithm 2.1 in which iterates have the form

\[ (3.1) \quad \begin{bmatrix} x_k \\ y_k \end{bmatrix} = W_k z_k, \]

where \( z_k \in \mathbb{R}^{2k} \) is defined by certain optimality properties. Thanks to (2.5) and (2.6), the residual of (1.1) at any iterate of the form (3.1) can be written

\[ r_k = \begin{bmatrix} b \\ c \end{bmatrix} - \begin{bmatrix} M & A \end{bmatrix} \begin{bmatrix} x_k \\ y_k \end{bmatrix} = H \begin{bmatrix} \beta_1 \\ \gamma_1 \end{bmatrix} - W_k S_{k+1} z_k = HW_{k+1}(\beta_1 e_1 + \gamma_1 e_2 - S_{k+1} z_k). \]

(3.2)

In the next few sections, the particular choice of \( z_k \) yields a simplified expression for the residual.

**3.1. Derivation of TriCG.** The \( k \)-th TriCG iterate has the form (3.1) with \( z_k \) defined by the Galerkin condition

\[ W_k^T r_k = 0 \quad \iff \quad W_k^T \begin{pmatrix} b \\ c \end{pmatrix} - \begin{bmatrix} M & A \end{bmatrix} \begin{bmatrix} x_k \\ y_k \end{bmatrix} = 0, \]

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which, thanks to (3.2), can be written as

\[ W_k^T H W_{k+1} (\beta_1 e_1 + \gamma_1 e_2 - S_{k+1,k} z_k) = 0. \]

By construction of the Krylov basis, \( W_k^T H W_k = I_{2k} \) and \( w_j^T H w_j = 0 \) for \( i \neq j \) in exact arithmetic. Let \( S_k \in \mathbb{R}^{2k \times 2k} \) denote the leading \((2k) \times (2k)\) submatrix of \( S_{k+1,k} \). This gives the TrICG subproblem:

(3.4) \[ S_k z_k = \beta_1 e_1 + \gamma_1 e_2. \]

### 3.1.1. Relation between TrICG and block-CG.

The \( k \)-th block-CG iterate is defined by the block-Galerkin condition

\[
W_k^T \left[ \begin{bmatrix} b & 0 \\ 0 & c \end{bmatrix} - \begin{bmatrix} M & A \\ A^T & -N \end{bmatrix} \right] \begin{bmatrix} x_k^b \\ y_k \end{bmatrix} = 0,
\]

where \((x_k^b, y_k) = W_k z_k^{b}\) and \((x_k^c, y_k^c) = W_k z_k^{c}\). Accordingly, the \( k \)-th block-CG subproblem is

(3.6) \[ S_k \begin{bmatrix} z_k^b \\ z_k^c \end{bmatrix} = [\beta_1 e_1 \, \gamma_1 e_2], \]

so that \( z_k^{b} \) and \( z_k^{c} \) solve the subproblem associated with right-hand sides \((b, 0)\) and \((0, c)\). The solutions of (3.4) and (3.6) are connected via \( z_k = z_k^{b} + z_k^{c} \), and the TrICG and block-CG approximations are connected via \( x_k = x_k^b + x_k^c \) and \( y_k = y_k^b + y_k^c \).

### 3.1.2. An LDL^T factorization.

The connection between Algorithm 2.1 and Algorithm 2.2 induces

(3.7) \[ S_k = P_k \begin{bmatrix} I_k & T_k \\ T_k^T & -I_k \end{bmatrix} P_k^T, \]

so that \( S_k \) is SQD, and therefore nonsingular, and (3.4) has a unique solution. Contrary to standard CG, the TrICG iterates are always well-defined. Vanderbei (1995) proved that SQD matrices are strongly factorizable, which means that, in particular, the factorization \( S_k = L_k D_k L_k^T \) where \( L_k \) is unit lower triangular and \( D_k \) is diagonal always exists. Subsequently, the solution \( z_k \) of (3.4) can be determined via forward and backward sweeps, although the next section shows that computing \( z_k \) is not necessary. The factorization of \( S_k \) can be updated at each iteration. Let

\[
D_k = \begin{bmatrix} d_1 & \cdots & \cdots \\ & \ddots & \cdots \\ & & d_{2k} \end{bmatrix}, \quad L_k = \begin{bmatrix} \Delta_1 \\ \Gamma_2 \\ \cdots \\ \Gamma_k \end{bmatrix}, \quad \Delta_k = \begin{bmatrix} 1 & 1 \\ \delta_k & 1 \end{bmatrix}, \quad \Gamma_k = \begin{bmatrix} \eta_k & \sigma_k \end{bmatrix}.
\]

If we initialize \( d_{-1} = d_0 = \sigma_1 = \eta_1 = \lambda_1 = 0 \), individual factorization steps are obtained from the recursion formulae

(3.8a) \[ d_{2k-1} = 1 - \sigma_k^2 d_{2k-2}, \quad k \geq 1, \]

(3.8b) \[ d_{2k} = -1 - \eta_k^2 d_{2k-3} - \lambda_k^2 d_{2k-2} - \delta_k^2 d_{2k-1}, \quad k \geq 1, \]

(3.8c) \[ \delta_k = (\alpha_k - \lambda_k \sigma_k d_{2k-2})/d_{2k-1}, \quad k \geq 1, \]

(3.8d) \[ \sigma_k = \beta_k/d_{2k-2}, \quad k \geq 2, \]

(3.8e) \[ \eta_k = \gamma_k/d_{2k-3}, \quad k \geq 2, \]

(3.8f) \[ \lambda_k = -\eta_k \delta_{k-1} d_{2k-3}/d_{2k-2}, \quad k \geq 2. \]
3.1.3. Update of the TrICG iterate. In order to compute the solution \( z_k \) of (3.4), we update the solution \( p_k := (\pi_1, \ldots, \pi_{2k}) \) of \( L_kD_kp_k = (\beta_1e_1 + \gamma_1e_2) \). The components of \( p_k \) are computed from

\[
\begin{align*}
(3.9a) \quad \pi_{2k-1} &= \begin{cases} 
\frac{\beta_1}{d_1}, & k = 1, \\
-\sigma_k d_{2k-2} \pi_{2k-2}/d_{2k-1}, & k \geq 2,
\end{cases} \\
(3.9b) \quad \pi_{2k} &= \begin{cases} 
(\gamma_1 - \delta_1 \pi_1)/d_2, & k = 1, \\
-(\delta_k d_{2k-1} \pi_{2k-1} + \lambda_k d_{2k-2} \pi_{2k-2} + \eta_k d_{2k-3} \pi_{2k-3})/d_{2k}, & k \geq 2.
\end{cases}
\end{align*}
\]

If we were to update \((x_k, y_k)\) directly from (3.1), all components of \( z_k := (\zeta_1, \ldots, \zeta_{2k}) \) would have to be recomputed because of the backward substitution required to solve \( L_k^T z_k = p_k \), which would require us to store \( W_k \) entirely. To avoid such drawbacks, we employ the strategy of Paige and Saunders (1975). Let

\[
(3.10) \quad G_k := W_k L_k^{-T} \iff L_k G_k^T = W_k^T, \quad G_k = \begin{bmatrix} G_k^x & G_k^y \end{bmatrix} = \begin{bmatrix} g_k^x & g_k^y \end{bmatrix},
\]

defined by \( g_k^x = g_0^x = g_1^x = 0 \), and the recursion

\[
\begin{align*}
g_{2k-1}^x &= -\sigma_k g_{2k-2}^x + v_k, \\
g_{2k-1}^y &= -\sigma_k g_{2k-2}^y, \\
g_{2k}^x &= -\delta_k g_{2k-1}^x - \lambda_k g_{2k-2}^x - \eta_k g_{2k-3}^x, \\
g_{2k}^y &= -\delta_k g_{2k-1}^y - \lambda_k g_{2k-2}^y - \eta_k g_{2k-3}^y + u_k.
\end{align*}
\]

This gives \((x_k, y_k) = W_k z_k = G_k L_k^T z_k = G_k p_k \) and the solution may be updated efficiently as

\[
\begin{align*}
x_k &= G_k^x p_k = x_{k-1} + \pi_{2k-1} g_{2k-1}^x + \pi_{2k} g_{2k}^x, \\
y_k &= G_k^y p_k = y_{k-1} + \pi_{2k-1} g_{2k-1}^y + \pi_{2k} g_{2k}^y.
\end{align*}
\]

3.1.4. Residual computation. The expression (3.2) combines with (3.4) to yield the residual at the TrICG iterate:

\[
\begin{align*}
r_k &= -H w_k (S_k z_k - \beta_1 e_1 - \gamma_1 e_2) - H w_{k+1} \Psi_{k+1}^T \begin{bmatrix} e_{2k-1}^T \\
\varepsilon_{2k}^T
\end{bmatrix} z_k \\
&= -H w_{k+1} \Psi_{k+1}^T \begin{bmatrix} \zeta_{2k-1} \\
\zeta_{2k}
\end{bmatrix} \\
&= -H w_{k+1} \begin{bmatrix} \beta_{k+1} \zeta_{2k} \\
\zeta_{2k} \zeta_{2k-1}
\end{bmatrix}.
\end{align*}
\]

Because \( L_k^T z_k = p_k \), we have \( \zeta_{2k} = \pi_{2k} \) and \( \zeta_{2k-1} = \pi_{2k-1} - \delta_k \pi_{2k} \). Therefore, with the relation \( w_{k+1} H w_{k+1} = I \), it is natural to measure the residual in the \( H^{-1} \)-norm:

\[
\begin{align*}
(3.14a) \quad \|r_0\|_{H^{-1}} &= \sqrt{\beta_1^2 + \gamma_1^2}, \\
(3.14b) \quad \|r_k\|_{H^{-1}} &= \sqrt{\beta_{k+1}^2 (\pi_{2k-1} - \delta_k \pi_{2k})^2 + \beta_{k+1}^2 \pi_{2k}^2}, \quad k \geq 1.
\end{align*}
\]

We summarize the complete procedure as Algorithm 3.1.
Algorithm 3.1 TriCG

Require: $A, b, c, v \mapsto M \setminus v, u \mapsto N \setminus u$

1. $x_0 = 0, y_0 = 0$
2. $g^z_0 = 0, g^y_0 = 0, g^x_0 = 0, g^y_0 = 0$
3. $u_0 = 0, v_0 = 0$
4. $\beta M v_1 = b, \gamma_1 N u_1 = c$
5. $||r_0||_H^{-1} = (\beta_1^2 + \gamma_1^2)^{1/2}$
6. $d_1 = 0 = \sigma_1 = \eta_1 = \lambda_1 = 0$
7. for $k = 1, 2, \ldots$ do
   8. $q = A u_k - \gamma_k M v_{k-1}, \alpha_k = v_k^T q$
   9. $p = A^T v_k - \beta_k N u_{k-1}$
   10. $\beta_{k+1} M v_{k+1} = q - \alpha_k M v_k$
   11. $\gamma_{k+1} N u_{k+1} = p - \alpha_k N u_k$
   12. $d_{2k-1} = 1 - \sigma_k^2 d_{2k-2}$
   13. $\delta_k = (\alpha_k - \lambda_k^2 \gamma_{2k-2}^2) / d_{2k-1}$
   14. $d_{2k} = -1 - \eta_k^2 d_{2k-3} - \lambda_k^2 d_{2k-2} - \delta_k^2 d_{2k-1}$
   15. if $k = 1$ then
      16. $\pi_{2k-1} = \beta_k / d_{2k-1}$
      17. $\pi_{2k} = (\gamma_k - \delta_k \beta_k) / d_{2k}$
   else
      19. $\sigma_k = \beta_k / d_{2k-2}$
      20. $\eta_k = \gamma_k / d_{2k-3}$
      21. $\lambda_k = - (\gamma_k \delta_{k-1} d_{2k-3}) / d_{2k-2}$
      22. $\pi_{2k-1} = -(\sigma_k \pi_{2k-2}^2 d_{2k-2}) / d_{2k-1}$
      23. $\pi_{2k} = - (\delta_k \pi_{2k-1} d_{2k-1} + \lambda_k \pi_{2k-2}^2 d_{2k-2} + \eta_k \pi_{2k-3} d_{2k-3}) / d_{2k}$
   end if
   25. $g^z_{2k-1} = v_k - \sigma_k g^z_{2k-2}$
   26. $g^z_{2k} = - \delta_k g^z_{2k-1} - \lambda_k g^z_{2k-2} - \eta_k g^z_{2k-3}$
   27. $g^y_{2k-1} = - \sigma_k g^y_{2k-2}$
   28. $g^y_{2k} = u_k - \delta_k g^y_{2k-1} - \lambda_k g^y_{2k-2} - \eta_k g^y_{2k-3}$
   29. $x_k = x_{k-1} + \pi_{2k-1} g^z_{2k-1} + \pi_{2k} g^z_{2k}$
   30. $y_k = y_{k-1} + \pi_{2k-1} g^y_{2k-1} + \pi_{2k} g^y_{2k}$
   31. $||r_k||_H^{-1} = (\gamma_{k+1} (\pi_{2k-1} - \delta_k \pi_{2k})^2 + \beta_{k+1}^2 \pi_{2k}^2)^{1/2}$
end for

3.1.5. Storage. TriCG requires one operator-vector product with $A$ and one with $A^T$ per iteration. With the assumption that in-place gemv updates of the form $y \leftarrow A u + g y$ and $y \leftarrow A^T v + \beta y$ are available, TriCG requires five $n$-vectors ($y_k, u_{k-1}, u_k, g^y_{2k-1}, g^y_{2k}$) and five $m$-vectors ($x_k, v_{k-1}, v_k, g^z_{2k-1}, g^z_{2k}$). If in-place gemv updates are not available, additional $m$- and $n$-vectors are required to store $Au$ and $A^T v$. Note that $A, A^T, M^{-1}$ and $N^{-1}$ do not need to be formed explicitly, and can be implemented as abstract operators. For instance, we could compute the Cholesky factorization of $M$ and $N$ and create abstract operators that perform the forward and backsolves. Extra $m$- and $n$-vectors could be necessary to store the results of those operators.

3.1.6. Properties. In this section, we formulate optimality properties of the TriCG iterates.
Proposition 3.1. The $k$-th TriCG iterate $(x_k, y_k)$ solves

\[
\begin{align*}
(3.15) \quad \min_{x \in \mathbb{R}^m} & \max_{y \in \mathbb{R}^n} \mathcal{L}(x, y) \\
\text{subject to} & \begin{bmatrix} x \\ y \end{bmatrix} \in \text{Range}(W_k),
\end{align*}
\]

where $\mathcal{L}(x, y) = \frac{1}{2} \|x\|_M^2 - \frac{1}{2} \|y\|_N^2 + x^T Ay - b^T x - c^T y$. Equivalently, $(x_k, y_k)$ solves

\[
(3.16) \quad \min_{x \in \mathbb{R}^m} \max_{y \in \mathbb{R}^n} \mathcal{E}(x, y) \quad \text{subject to} \quad \begin{bmatrix} x \\ y \end{bmatrix} \in \text{Range}(W_k),
\]

where $\mathcal{E}(x, y)$ is the indefinite error metric

\[
\mathcal{E}(x, y) := e^T \begin{bmatrix} M & A \\ A^T & -N \end{bmatrix} e_r, \quad e_r := (x^* - x, \ y^* - y),
\]

and $(x^*, y^*)$ is the exact solution of (1.1).

Proof. $\mathcal{L}(x, y)$ is strictly convex in $x$ because $\nabla^2_{xx} \mathcal{L}(x, y) = M \succ 0$ and strictly concave in $y$ because $\nabla^2_{yy} \mathcal{L}(x, y) = -N \prec 0$. Therefore, (3.15) admits a unique solution because the feasible set $\text{Range}(W_k) \neq \emptyset$. Its first-order optimality conditions are

\[
W_k^T \begin{bmatrix} Mx + Ay - b \\ A^T x - Ny - c \end{bmatrix} = 0,
\]

and coincide with (3.3). The rest of the proof follows from the fact that $\mathcal{L}(x, y)$ and $\mathcal{E}(x, y)$ are equal up to a constant. □

Although SQD matrices are indefinite, $\mathcal{E}(x, y)$ can be seen as a metric that generalizes the energy norm. A similar metric is used by Orban and Arioli (2017) in the context of their generalized conjugate gradient method for SQD systems. Figure 3.1 illustrates the evolution of $\mathcal{E}(x_k, y_k)$ along the TriCG iterations on problem illc1850, to be described in section 4, where oscillations from positive to negative values and decreasing amplitude are evident.

![Figure 3.1](image-url)
3.2. Derivation of TriMR. In the same way as TriCG is related to block-Cg, the minimum residual variant TriMR developed below is related to block-MNRES. The \( k \)-th TriMR iterate is defined as the solution of the linear least-squares problem

\[
\min_{(z_k,y_k) \in \text{Range}(W_k)} \| r_k \|_{H^{-1}} \quad \iff \quad \min_{z_k \in \mathbb{R}^{2k}} \| S_{k+1,k} z_k - \beta_1 e_1 - \gamma_1 e_2 \|,
\]

where the equivalence follows from (3.2). We now outline the main stages of the subproblem solution.

3.2.1. A QR factorization. The solution of (3.17) can be determined via the QR factorization

\[
S_{k+1,k} = Q_k \begin{bmatrix} R_k & \end{bmatrix},
\]

which can be updated at each iteration, where \( Q_k \in \mathbb{R}^{(2k+2) \times (2k+2)} \) is a product of Givens reflections, and

\[
R_k = \begin{bmatrix}
\delta_1 & \sigma_1 & \eta_1 & \lambda_1 & \mu_1 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
& & & & \\
\mu_{2k-4} & \lambda_{2k-3} & \eta_{2k-2} & \sigma_{2k-1} & \delta_{2k}
\end{bmatrix} \in \mathbb{R}^{(2k) \times (2k)}.
\]

Below, we outline the main steps of the update and commit all details to Appendix B for reference.

At iteration \( k \), four reflections are necessary to update (3.18). Together, they affect four rows and six columns of \( S_{k+1,k} \). We denote their product \( Q_{2k-1,2k+2} \) in (B.1) so that \( Q_k^T = Q_{2k-1,2k+2} \cdots Q_{1,4} \). If we initialize \( \tilde{\theta}_1 := \alpha_1, \tilde{\delta}_1 := 1, \tilde{\delta}_2 := -1, \tilde{\sigma}_1 := \alpha_1, \tilde{\eta}_1 := 0, \tilde{\lambda}_1 := \gamma_2 \) and \( \tilde{\sigma}_2 := \beta_2 \), individual factorization steps may be represented as an application of \( Q_{2k-1,2k+2} \) to \( Q_{k-1} S_{k+1,k} \):

\[
\begin{bmatrix}
2k-1 & 2k \\
2k & 2k+1 & 2k+2 & 2k+3 & 2k+4 \\
2k+1 & 0 & \gamma_{k+1} & 1 & \alpha_{k+1} & 0 & \gamma_{k+2} \\
2k+2 & \beta_{k+1} & 0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0
\end{bmatrix}.
\]

Because \( \alpha_{k+1}, \gamma_{k+2} \) and \( \beta_{k+2} \) are not yet available at iteration \( k \), we apply the last four reflections at iteration \( k + 1 \) to determine all remaining coefficients of rows \( 2k-1 \) and \( 2k \) of \( R_{k+1} \) and \( R_{k+2} \):

\[
\begin{bmatrix}
2k-1 & 2k \\
2k & 2k+1 & 2k+2 & 2k+3 & 2k+4 \\
2k+1 & 0 & \delta_{2k-1} & \sigma_{2k-1} & \eta_{2k-1} & \lambda_{2k-1} & 0 \\
2k+2 & 0 & \delta_{2k} & \sigma_{2k} & \eta_{2k} & \lambda_{2k} & \mu_{2k}
\end{bmatrix}.
\]

Additional details about the four reflections that compose \( Q_{2k-1,2k+4} \) and the factorization are available in (B.2)–(B.5).

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3.3. Update of the TriMR iterate. We can avoid computing $z_k$ in (3.17) for the same reasons as with TriCG by updating instead $p_k := (\pi_1, \ldots, \pi_{2k})$, which is defined via $R_k z_k = p_k$:

\begin{align}
&\bar{p}_0 := (\beta_1, \gamma_1), \\
&\bar{p}_k := (p_k, \bar{\pi}_{2k+1}, \bar{\pi}_{2k+2}) = Q_k^T (\beta_1 e_1 + \gamma_1 e_2), \quad k \geq 1.
\end{align}

$p_k$ can be easily determined from $\bar{p}_{k-1}$ because $\bar{p}_k = Q_{2k-1,2k+2} (\bar{p}_{k-1}, 0, 0)$. Details are given in (B.6) and (B.7). We set

\begin{equation}
G_k := W_k R_k^{-1} \iff R_k G_k^T = W_k^T,
\end{equation}

similarly to (3.10). The columns of $G_k$ are obtained from the recursion

\begin{align}
g_{2k-1}^x &= (v_k - \mu_{2k-5} g_{2k-5}^x - \lambda_{2k-4} g_{2k-4}^x - \eta_{2k-3} g_{2k-3}^x - \sigma_{2k-2} g_{2k-2}^x - 2 g_{2k-2}^y)/\delta_{2k-1} \\
&= (v_k - \mu_{2k-5} g_{2k-5}^x - \lambda_{2k-4} g_{2k-4}^x - \eta_{2k-3} g_{2k-3}^x - \sigma_{2k-2} g_{2k-2}^y)/\delta_{2k-1} \\
g_{2k}^x &= (v_k - \mu_{2k-4} g_{2k-4}^x - \lambda_{2k-3} g_{2k-3}^x - \eta_{2k-2} g_{2k-2}^x - \sigma_{2k-1} g_{2k-1}^y)/\delta_{2k} \\
g_{2k}^y &= (u_k - \mu_{2k-4} g_{2k-4}^y - \lambda_{2k-3} g_{2k-3}^y - \eta_{2k-2} g_{2k-2}^y - \sigma_{2k-1} g_{2k-1}^y)/\delta_{2k},
\end{align}

where we set $\eta_j$, $\lambda_j$, $\mu_j$, $g_j^x$ and $g_j^y$ to zero if $j \leq 0$. Analogously to TriCG, $(x_k, y_k) = W_k z_k = G_k R_k z_k = G_k p_k$ and the solution may be updated efficiently as (3.12).

3.3.1. Residual computation. The definition of $\bar{p}_k$, (3.2) and (3.18) yield

\begin{equation}
\|r_k\|_{H^{-1}} = \|S_{k+1,k} z_k - (\beta_1 e_1 + \gamma_1 e_2)\| = \sqrt{\|R_k z_k - \bar{p}_k\|^2} = \sqrt{\pi_{2k+1}^2 + \pi_{2k+2}^2}.
\end{equation}

The complete algorithm is stated as Algorithm 3.2.

3.3.2. Storage. TriMR has the same storage requirements as TriCG plus two $n$-vectors ($g_{2k-2}^x$, $g_{2k-3}^y$) and two $m$-vectors ($g_{2k-2}^x$, $g_{2k-3}^y$). All other vectors are identical to those in TriCG.

4. Implementation and numerical experiments. We evaluate the performance of TriCG and TriMR on SQD systems generated from rectangular matrices $A$ obtained from the UFL collection of Davis and Hu (2011).\footnote{Now the SuiteSparse Matrix Collection \url{sparse.tamu.edu}.} We implemented Algorithm 3.1 and Algorithm 3.2 in Julia\footnote{\url{julialang.org}} (Bezanson, Edelman, Karpinski, and Shah, 2017), version 1.5. Both algorithms are available as part of the Krylov.jl collection of Krylov methods (Monteison, Orban, and contributors, 2020).

Because standard CG may break down when applied to (1.1), we compare the evolution of the TriCG residual to that of SYMMLQ, whose iterates are always well defined. Similarly, we compare the evolution of the TriMR residual to that of MINRES. In order to evaluate benefits of TriCG and TriMR in terms of loss of orthogonality along the iterations, we also compare the evolution of TriCG and TriMR residuals to those of BLock-CG and BLock-MINRES, respectively, applied to $K$ with block right-hand side $B$ where the two approximate solutions are summed at the last iteration.

SYMMLQ, BLock-CG, MINRES and BLock-MINRES are run with preconditioner $H$.

In our first set of experiments, we set $M$ and $N$ to the identity. Thus the $H^{-1}$-norm is simply the Euclidean norm. The right-hand side $(b,c)$ is generated such
Algorithm 3.2 TriMR

Require: $A, b, c, v \mapsto M \setminus v, u \mapsto N \setminus u$

1: $x_0 = 0, y_0 = 0$
2: $g^x_{-2} = 0, g^y_{-2} = 0, g^z_{-1} = 0, g^u_0 = 0$
3: $g^x_{-3} = 0, g^y_{-2} = 0, g^y_{-1} = 0, g^y_0 = 0$
4: $u_0 = 0, v_0 = 0$
5: $\beta_1 M v_1 = b, \gamma_1 N u_1 = c$
6: $\|r_0\|_{H^{-1}} = \left(\beta_1^2 + \gamma_1^2\right)^{\frac{1}{2}}$
7: for $k = 1, 2, \ldots$ do
8: \begin{align*}
q &= Au_k - \gamma_k M v_{k-1}, \alpha_k = v^T_k q \\
p &= A^T v_k - \beta_k N u_{k-1}
\end{align*}
9: $\beta_{k+1} M v_{k+1} = q - \alpha_k M v_k$
10: $\gamma_{k+1} N u_{k+1} = p - \alpha_k N u_k$
11: if $k = 1$ then
12: \begin{align*}
\bar{\theta}_1 &= \alpha_1, \bar{\delta}_1 = 1, \bar{\delta}_2 = -1 \\
\bar{\bar{\sigma}}_1 &= \alpha_1, \bar{\bar{\eta}}_1 = 0, \bar{\bar{\lambda}}_1 = \beta_2, \bar{\bar{\sigma}}_2 = \gamma_2
\end{align*}
13: else
14: Compute $\eta_{2k-3}, \lambda_{2k-3}, \mu_{2k-3}, \sigma_{2k-2}, \eta_{2k-2}, \lambda_{2k-2}, \mu_{2k-2}, \sigma_{2k-2}$ update $R_k$
15: Compute $\theta_{2k}, \delta_{2k-1}, \delta_{2k}, \sigma_{2k-1}, \eta_{2k-1}, \lambda_{2k-1}, \sigma_{2k}$ update $R_k$
16: Compute $Q_{2k-1,2k+2}, \delta_{2k-1}, \sigma_{2k-1}, \delta_{2k}$ continue the QR factorization
17: Compute $\pi_{2k-1}, \bar{\pi}_{2k+1}, \bar{\bar{\pi}}_{2k+2}$ update $\pi_k$
18: $g^x_{2k-1} = (v_k - \mu_{2k-5} g^x_{2k-5} - \lambda_{2k-4} g^y_{2k-4} - \eta_{2k-3} g^z_{2k-3} - \sigma_{2k-2} g^u_{2k-2})/\delta_{2k-1}$
19: $g^y_{2k} = -\left((\mu_{2k-5} g^x_{2k-5} + \lambda_{2k-4} g^y_{2k-4} + \eta_{2k-3} g^z_{2k-3} + \sigma_{2k-2} g^u_{2k-2})/\delta_{2k-1}\right)$ update $G^x_k$
20: $g^y_{2k-1} = -\left((\mu_{2k-5} g^x_{2k-5} + \lambda_{2k-4} g^y_{2k-4} + \eta_{2k-3} g^z_{2k-3} + \sigma_{2k-2} g^u_{2k-2})/\delta_{2k-1}\right)$ update $G^y_k$
21: $g^z_{2k} = (v_k - \mu_{2k-4} g^x_{2k-4} - \lambda_{2k-3} g^y_{2k-3} - \eta_{2k-2} g^z_{2k-2} - \sigma_{2k-1} g^u_{2k-1})/\delta_{2k}$ update $G^z_k$
22: $x_k = x_{k-1} + \bar{\pi}_{2k-1} g^x_{2k-1} + \bar{\bar{\pi}}_{2k+2} g^y_{2k}$
23: $y_k = y_{k-1} + \bar{\pi}_{2k-1} g^y_{2k-1} + \bar{\bar{\pi}}_{2k+2} g^y_{2k}$
24: $r_k = \|r_k\|_{H^{-1}} = \left(\bar{\pi}_{2k+1}^2 + \bar{\bar{\pi}}_{2k+2}^2\right)^{\frac{1}{2}}$ compute $\|r_k\|_{H^{-1}}$
25: end for

that the exact solution of (1.1) is the vector of ones. Residuals $r_k = b - Ax_k$ are calculated explicitly at each iteration in order to evaluate $\|r_k\|$ instead of using (3.13) or (3.23). Each algorithm stops as soon as $\|r_k\| \leq \varepsilon_a + \|(b,c)\| \varepsilon_r$ with absolute tolerance $\varepsilon_a = 10^{-12}$ and relative tolerance $\varepsilon_r = 10^{-10}$.

Figures 4.1 and 4.2 report residual histories on matrices arising from linear optimization. In all cases, the TriCG and TriMR residuals attain the required tolerance in around half the number of iterations of SYMMLQ and MINRES, respectively. We also note that the TriCG and BLOCK-CG residuals are close, but not quite superposed, as are the MINRES and BLOCK-MINRES residuals. These results are encouraging if one wishes to employ TriCG or TriMR to solve the linear systems emerging at each iteration of a numerical method for constrained optimization, including interior-point methods, where the systems have the form of those just tested. The results also suggest that orthogonality is not lost quite as fast in TriCG and TriMR as it is in BLOCK-CG and BLOCK-MINRES.

Figures 4.3 and 4.4 report residual histories on matrices arising from least-squares problems. In all cases, TriCG and TriMR require fewer iterations than SYMMLQ and MINRES. On these two problems, the residuals of the block methods are nearly
superposed. We observe on our test problems that TriCG and TriMR perform fewer iterations when the singular values of $A$ are clustered. However, a deeper analysis is required to confirm this empirical observation.

We simulate the behavior of the six methods in exact arithmetic in hopes to compare loss of orthogonality empirically. Figure 4.5 reports residual histories obtained...
when running each method on $lp\_osa\_07$ entirely in quadruple and octuple precision, and should be compared with Figure 4.2. This time, the TriCG and BLOCK-Cg residuals are nearly superposed, as are the TriMR and BLOCK-MINRES residuals as the increased accuracy of arithmetic mitigates loss of orthogonality. The block methods continue to require around half as many iterations as the standard methods. However, we note an additional phenomenon: doubling the number of digits reduces the number of iterations by a factor of approximately two.

**Fig. 4.4.** Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR on landmark, where $A$ is $71952 \times 2704$ with 1146848 nonzeros.

**Fig. 4.5.** Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR iterates on $lp\_osa\_07$ in quadruple (top) and octuple precision (bottom).

In a second set of experiments, we run all six methods on discretized and stabilized
Stokes equations generated by the MATLAB package IFISS, version 3.6, of Elman, Ramage, and Silvester (2019). Whenever the discrete velocity and pressure belong to finite-element spaces that do not satisfy the inf-sup, or Ladyzhenskaya-Babuška-Brezzi (LBB), stability conditions (Boffi, Brezzi, and Fortin, 2013), a nonzero and negative semi-definite stabilization term $-N$ is inserted in the bottom block of (1.6). It is the case with the unstable 2D finite-element pairs $Q_1-P_0$ and $Q_1-Q_1$, which we use on a test problem from IFISS. In order to obtain an SQD system, we add $10^{-5}I$ to $N$. For this set of problems, $M$ and $N$ are not identity operators, and each algorithm stops as soon as $\|r_k\|_{H^{-1}} \leq \varepsilon_a + \|(b, c)\|_{H^{-1}} \varepsilon_r$ with the same tolerances as above.

Fig. 4.6. Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR on channel_domain problem with $Q_1-P_0$ discretization. The discretized linear system has size $12546 \times 12546$ with 147742 nonzeros.

Fig. 4.7. Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR on channel_domain problem with $Q_1-Q_1$ discretization. The discretized linear system has size $12675 \times 12675$ with 242381 nonzeros.

Figures 4.6 and 4.7 report residual histories. TriCG and TriMR reach the prescribed tolerance before Symmlq and Minres with around 25% fewer iteration. These results suggest that TriCG and TriMR may be of interest to solve other PDEs whose discretization leads to (1.1), such as the Reissner-Mindlin plate model in linear elasticity (Braess, 2007).
4.1. Discussion and extensions. Although we develop TriCG and TriMR for SQD systems, both can be generalized to handle any linear system of the form

$$\begin{bmatrix} \pm M & A \\ A^T & \pm N \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix},$$

where $M$ and $N$ are symmetric positive definite. Symmetric definite systems can always be written in the form (4.1). For instance, one could solve any definite system by first partitioning any symmetric permutation of it as (4.1) and applying TriCG or TriMR to the resulting $A$. There are multiple ways to perform such partitioning, and it is not clear whether such strategy might lead to improved solution processes for SPD systems. With minor modifications, TriMR also supports the saddle-point system (1.6). In this case, $N$ can be replaced by any SPD matrix to define an elliptic norm in Algorithm 2.1, which extends the possibilities for preconditioning the linear system. For instance, TriMR could use the preconditioner $\text{blkdiag}(M, S)$ (Murphy, Golub, and Wathen, 2000) for Stokes problems discretized by LBB-stable finite element pairs where $S$ is the Schur complement $A^T M^{-1} A$ or an approximation to it. Our implementations of TriCG and TriMR take into account all these extensions, are applicable in any floating-point system supported by Julia, and run on GPUs.

TriCG and TriMR perform substantially better than SYMMLQ and MINRES in our experiments and often terminate in about half as many iterations on a residual-based stopping condition. Nevertheless more extensive testing is required to properly assess their performance in practice. Although theoretically equivalent, TriCG and TriMR appear to preserve orthogonality of the Krylov basis better than their counterparts Block-CG and Block-MINRES. Additional numerical illustrations are available in Appendix A.

Based upon Algorithm 2.1, it is possible to develop a third method in the spirit of SYMMLQ that we could name TriLQ. The TriLQ subproblem selects $z_k$ in (3.1) as the solution of the minimum-norm subproblem

$$\min_{z_k \in \mathbb{R}^{2k}} \|z_k\| \quad \text{subject to} \quad S_{k-1,k} z_k = \beta_1 e_1 + \gamma_1 e_2,$$

where $S_{k-1,k}$ is the leading $(2k-2) \times (2k)$ submatrix of $S_{k+1,k}$ in (2.6). The subproblem can be solved via the LQ factorization of $S_{k-1,k}$. Much of TriLQ would be similar to block-SYMMQL: iterates are updated along orthogonal directions, the $H$-norm of the iterates increases monotonically, and the $H$-norm of the error decreases monotonically. At each iteration, TriLQ allows the user to transfer to the TriCG iterate. Because the TriCG iterate always exists for (1.1), TriLQ might not have have any advantage in practice, other than completing the family of numerical methods based on Algorithm 2.1. However, the TriLQ iterate remains well defined for the saddle-point system (1.6), whereas TriCG may break down in that case.

The strong connection between TriCG and block-CG with blocks of size 2 suggests that TriCG might also be useful to approximate eigenvalues. We leave the investigation of such extensions to future work.

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Appendix A. Additional numerical results.

This appendix contains further numerical comparisons between TriCG, TriMR, BLOCK-Cg, BLOCK-Minres, SYMMdq and MINRES. Figure A.1 reports residual histories in double precision on another underdetermined system from optimization, where BLOCK-Cg and BLOCK-MINRES do not converge, presumably due to excessive loss of orthogonality. Figure A.2 corresponds to a well-conditioned overdetermined system from a least-squares application, where the residuals of the block methods nearly coincide. Figures A.3 and A.4 are Stokes systems. Finally, Figure A.5 is a rather dramatic example of an underdetermined system from optimization where only TriCG and TriMR converge in double precision. As the accuracy increases, BLOCK-Cg and BLOCK-MINRES converge and nearly coincide with TriCG and TriMR. Moreover, as the number of digits doubles, the number of iterations to converge is roughly halved.

Fig. A.1. Residual history of SYMMdq, BLOCK-Cg, TriCG, Minres, BLOCK-Minres and TriMR on lp_d6cube, where $A$ is $415 \times 6184$ with $37704$ nonzeros.

Fig. A.2. Residual history of SYMMdq, BLOCK-Cg, TriCG, Minres, BLOCK-Minres and TriMR on well1033, where $A$ is $1033 \times 320$ with $4732$ nonzeros.
Fig. A.3. Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR iterates on colliding_flow problem with $Q_1 - P_0$ discretization. The discretized linear system has size $12546 \times 12546$ with 146241 nonzeros.

Fig. A.4. Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR iterates on colliding_flow problem with $Q_1 - Q_1$ discretization. The discretized linear system has size $12675 \times 12675$ with 239873 nonzeros.
Fig. A.5. Residual history of Symmlq, Block-Cg, TriCG, Minres, Block-Minres and TriMR iterates on lpi_klein3 in double (top), quadruple (center) and octuple precision (bottom) where \( A \) is 994 x 1082 with 13101 nonzeros.
Appendix B. TrIMR details.

\( Q_{2k-1,2k+2} := \begin{bmatrix}
1 & c_{4,k} & s_{4,k} \\
1 & c_{3,k} & s_{3,k} \\
1 & c_{2,k} & s_{2,k} \\
1 & c_{1,k} & s_{1,k}
\end{bmatrix} \begin{bmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 0
\end{bmatrix} \begin{bmatrix}
s_{4,k} & -c_{4,k} \\
s_{3,k} & -c_{3,k} \\
s_{2,k} & -c_{2,k} \\
s_{1,k} & -c_{1,k}
\end{bmatrix} \)

(B.1)

\[
\begin{pmatrix}
\delta_{2k-1} & \sigma_{2k-1} & \eta_{2k-1} & \lambda_{2k-1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix}
= \begin{pmatrix}
\delta_{2k-1} & \sigma_{2k-1} & \eta_{2k-1} & \lambda_{2k-1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix} = \begin{pmatrix}
\delta_{2k+1} & \sigma_{2k+1} & \eta_{2k+1} & \lambda_{2k+1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix}
\]

(B.2a)

\[
\theta_k = \sqrt{\sigma_k^2 + \beta_k^2}, \quad c_{1,k} = \theta_k / \lambda_k, \quad s_{1,k} = \beta_k / \lambda_k
\]

(B.2b)

\[
\tilde{\delta}_k = c_{1,k} \tilde{\delta}_k, \quad \tilde{\sigma}_k = c_{1,k} \tilde{\sigma}_k + s_{1,k} \alpha_{k+1}, \quad \tilde{\eta}_k = -s_{1,k}, \quad \tilde{\lambda}_k = s_{1,k} \beta_{k+2}, \quad \tilde{\sigma}_{2k+2} = -c_{1,k} \beta_{k+2}.
\]

(B.2c)

\[
\begin{pmatrix}
\delta_{2k-1} & \sigma_{2k-1} & \eta_{2k-1} & \lambda_{2k-1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix}
= \begin{pmatrix}
\delta_{2k-1} & \sigma_{2k-1} & \eta_{2k-1} & \lambda_{2k-1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix} = \begin{pmatrix}
\delta_{2k+1} & \sigma_{2k+1} & \eta_{2k+1} & \lambda_{2k+1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix} = \begin{pmatrix}
\delta_{2k+1} & \sigma_{2k+1} & \eta_{2k+1} & \lambda_{2k+1} & 0 & 0 \\
\theta_k & \delta_{2k} & \sigma_{2k} & \eta_{2k} & 0 & 0 \\
0 & \gamma_{k+1} & \alpha_{k+1} & 0 & \gamma_{k+2} & 0 \\
0 & \alpha_{k+1} & -1 & \beta_{k+2} & 0 & 0
\end{pmatrix}
\]

(B.3a)

\[
\delta_{2k-1} = \sqrt{\delta_{2k-1}^2 + \theta_k^2}, \quad c_{2,k} = \delta_{2k-1}/\delta_{2k-1}, \quad s_{2,k} = \theta_k/\delta_{2k-1}
\]
(B.3b) \[ \sigma_{2k-1} = c_{2,k} \bar{\sigma}_{2k-1} + s_{2,k} \bar{\sigma}_{2k}, \]
\[ \eta_{2k-1} = c_{2,k} \bar{\eta}_{2k-1} + s_{2,k} \bar{\sigma}_{2k}, \]
\[ \lambda_{2k-1} = c_{2,k} \bar{\lambda}_{2k-1} + s_{2,k} \bar{\eta}_{2k}, \]
\[ \mu_{2k-1} = s_{2,k} \bar{\lambda}_{2k}. \]
\[ \bar{\delta}_{2k} = s_{2,k} \bar{\sigma}_{2k-1} - c_{2,k} \bar{\delta}_{2k}, \]
\[ \bar{\sigma}_{2k} = s_{2,k} \bar{\eta}_{2k-1} - c_{2,k} \bar{\sigma}_{2k}, \]
\[ \bar{\eta}_{2k} = s_{2,k} \bar{\lambda}_{2k-1} - c_{2,k} \bar{\eta}_{2k}, \]
\[ \bar{\lambda}_{2k} = -c_{2,k} \bar{\lambda}_{2k}. \]

\[ \delta_{2k} = \sqrt{\delta_{2k}^2 + g_{k}^2}, \quad c_{3,k} = \frac{\delta_{2k}}{\delta_{2k}}, \quad s_{3,k} = g_{k}/\delta_{2k} \]

(B.4a) \[ \bar{\delta}_{2k} = \sqrt{\delta_{2k}^2 + g_{k}^2}, \quad c_{3,k} = \frac{\delta_{2k}}{\delta_{2k}}, \quad s_{3,k} = g_{k}/\delta_{2k} \]

(B.4b) \[ \bar{\sigma}_{2k} = c_{3,k} \bar{\sigma}_{2k} + s_{3,k} \bar{\theta}_{k+1}, \]
\[ \bar{\eta}_{2k} = c_{3,k} \bar{\eta}_{2k} + s_{3,k} \bar{\sigma}_{2k+2}, \]
\[ \bar{\lambda}_{2k} = c_{3,k} \bar{\lambda}_{2k} + s_{3,k} \bar{\sigma}_{2k+2}, \]
\[ \bar{\theta}_{k+1} = s_{3,k} \bar{\sigma}_{2k} - c_{3,k} \bar{\theta}_{k+1}, \]
\[ \bar{\eta}_{2k+2} = s_{3,k} \bar{\eta}_{2k} - c_{3,k} \bar{\eta}_{2k+2}, \]
\[ \bar{\lambda}_{2k+2} = s_{3,k} \bar{\lambda}_{2k} - c_{3,k} \bar{\lambda}_{2k+2}. \]

(B.5a) \[ \delta_{2k} = \sqrt{\delta_{2k}^2 + \gamma_{k+1}^2}, \quad c_{4,k} = \frac{\delta_{2k}}{\delta_{2k}}, \quad s_{4,k} = \gamma_{k+1}/\delta_{2k} \]

(B.5b) \[ \bar{\sigma}_{2k} = c_{4,k} \bar{\sigma}_{2k} + s_{4,k}, \]
\[ \bar{\eta}_{2k} = c_{4,k} \bar{\eta}_{2k} + s_{4,k} \bar{\lambda}_{k+1}, \]
\[ \bar{\lambda}_{2k} = c_{4,k} \bar{\lambda}_{2k}, \]
\[ \bar{\delta}_{2k+1} = s_{4,k} \bar{\sigma}_{2k} - c_{4,k}, \]
\[ \bar{\eta}_{2k+1} = s_{4,k} \bar{\lambda}_{k+1}. \]

(B.5c) \[ \bar{\theta}_{2k+1} = s_{4,k} \bar{\theta}_{2k} - c_{4,k}, \]
\[ \bar{\eta}_{2k+1} = s_{4,k} \bar{\lambda}_{2k}, \]
\[ \bar{\lambda}_{2k+1} = -c_{4,k} \gamma_{k+2}. \]
Scalars decorated by a hat, a tilde or a ring are updated at the current iteration. Scalars decorated by a bar will be updated at the next iteration. Scalars without any decoration have been updated to their final value.