A MODIFIED IMPLEMENTATION OF MINRES TO MONITOR RESIDUAL SUBVECTOR NORMS FOR BLOCK SYSTEMS

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Abstract. Saddle-point systems, i.e., structured linear systems with symmetric matrices are considered. A modified implementation of (preconditioned) MINRES is derived which allows to monitor the norms of the subvectors individually. Compared to the implementation from the textbook of [Elman, Sylvester and Wathen, Oxford University Press, 2014], our method requires one extra vector of storage and no additional applications of the preconditioner. Numerical experiments are included.

Key words. MINRES, saddle-point problems, structured linear systems, preconditioning, sub-vector norms

AMS subject classifications. 65F08, 65F10, 15B57, 65M22, 74S05, 76M10

1. Introduction. We are solving symmetric linear systems of the form

\[
\begin{bmatrix}
A & B^T \\
B & -C
\end{bmatrix}
\begin{bmatrix}
u \\
p
\end{bmatrix}
=
\begin{bmatrix}
f_u \\
f_p
\end{bmatrix},
\]

where \(A \in \mathbb{R}^{m \times m}\) and \(C \in \mathbb{R}^{p \times p}\) are symmetric, and \(B \in \mathbb{R}^{p \times m}\), by applying MINRES or preconditioned MINRES [8] iteration. After \(j\) iterations, we have approximation \((u^{(j)}, p^{(j)})\) and residual

\[
r^{(j)} = \begin{bmatrix} f_u \\ f_p \end{bmatrix} - \begin{bmatrix} A & B^T \\
B & -C \end{bmatrix} \begin{bmatrix} u^{(j)} \\ p^{(j)} \end{bmatrix} = \begin{bmatrix} f_u \\ f_p \end{bmatrix} - \begin{bmatrix} Au^{(j)} + B^T p^{(j)} \\
Bu^{(j)} - Cp^{(j)} \end{bmatrix}.
\]

We denote the two parts of the residual as

\[
r_u^{(j)} = f_u - (Au^{(j)} + B^T p^{(j)}) \quad \text{and} \quad r_p^{(j)} = f_p - (Bu^{(j)} - Cp^{(j)}).
\]

The question we seek to answer is: can we monitor the individual preconditioned norms of \(r_u^{(j)}\) and \(r_p^{(j)}\) (as opposed to the full norm of \(r^{(j)}\)) using only quantities arising in an efficient implementation of the preconditioned MINRES algorithm, namely that in [2, Algorithm 4.1]? The answer is yes, under certain conditions. The technical requirements to do so are connected to the notion of so-called “natural” preconditioners which arise in this setting; see, e.g., [9, 12] and references contained therein. In section 2, we demonstrate that at the storage cost of one additional full-length vector and six scalars but no additional applications of the preconditioner, one can modify the preconditioned MINRES method to calculate these norms in a progressive fashion. An extension to more than two residual parts is straightforward. An implementation of our modified version of MINRES is given in algorithm 1 and is available at [6] as a Matlab file.

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As a motivation for our study, we mention that the individual parts of the residual in (1.1) often have different physical interpretations. Monitoring them individually allows a better insight into the convergence of MINRES and it allows the formulation of refined stopping criteria. We present examples and numerical experiments in section 3.

2. How to monitor both parts of the preconditioned residual. In this section, we derive how one monitors these norms without incurring much extra computational or storage expense. We will describe everything in terms of the variable names used in [2, Algorithm 4.1] with two exceptions, which will be noted below.

Here we describe quickly the derivation of preconditioned MINRES as a Krylov subspace method, specifically in order to relate certain quantities from [2, Algorithm 4.1] to the common quantities arising in the Lanczos process. In principle, the preconditioned MINRES algorithm is an implementation of the minimum residual Krylov subspace method for matrices which are symmetric. It can be equivalently formulated as an iteration for operator equations in which the operator is self-adjoint, mapping elements of a Hilbert space into its dual; see [5]. We present the derivation for the finite dimensional case. For the purposes of this discussion, let $x^{(j)} = (u^{(j)}, p^{(j)})$ be the $j$th approximation. Let $P = \begin{bmatrix} P_u & P_p \end{bmatrix}$ with $P_u \in \mathbb{R}^{m \times m}$ and $P_p \in \mathbb{R}^{p \times p}$.

This assumption is natural in many situations when we acknowledge that the residual subvectors often have different physical meaning and need to be measured in different norms; see [9, 12] and section 3 for examples.

We briefly review some basic facts about Krylov subspaces for symmetric matrices. We begin with the unpreconditioned situation. Let $A \in \mathbb{R}^{n \times n}$ be symmetric. For some starting element $h \in \mathbb{R}^n$, we define the $j$th Krylov subspace generated by $A$ and $h$ to be

$$K_j(A, h) = \text{span} \{ h, Ah, A^2h, \ldots, A^{j-1}h \}$$

using the Lanczos process, where if $V_j = \begin{bmatrix} v_1 & v_2 & \cdots & v_j \end{bmatrix} \in \mathbb{R}^{n \times j}$ is the matrix with columns that form an orthonormal basis of $K_j(A, h)$, then we have the Lanczos relation

$$AV_j = V_{j+1}T_j \quad \text{where} \quad T_j \in \mathbb{R}^{(j+1) \times j}.$$  

The matrix $T_j$ is tridiagonal, and the matrix $T_j$ (defined as the first $j$ rows of $T_j$) is symmetric. This implies that to generate each new Lanczos vector, we must orthogonalize the newest vector against only the two previous Lanczos vectors. This leads to the following well-known three-term recurrence formula

$$Av_j = \gamma_{j+1}v_{j+1} + \delta_j v_j + \gamma_j v_{j-1}.$$

Using the naming conventions in [2, Algorithm 2.4], we have

\[
T_j = \begin{bmatrix}
\delta_1 & \gamma_2 & \ldots & \ldots & \gamma_j \\
\gamma_2 & \ddots & \ddots & \ddots & \gamma_j \\
\vdots & \ddots & \ddots & \ddots & \gamma_j \\
\gamma_j & \ldots & \ldots & \ddots & \gamma_{j+1}
\end{bmatrix}.
\]

In the case that we have a symmetric positive definite preconditioner \(P\), we show that a Krylov subspace can still constructed using the short-term Lanczos iteration and that a MINRES method can be used for solving (1.1). In, e.g., [2], preconditioned MINRES is derived by first observing that \(P\) admits the Cholesky decomposition \(P = HH^T\). Thus one could consider solving the two-sided preconditioned equations

\[
H^{-1}KH^{-T}y = H^{-1}b \quad \text{with} \quad y = H^Tx \quad \text{where} \quad x = \begin{bmatrix} u \\ p \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},
\]

where we have the initial approximation \(y^{(0)} = H^Tx^{(0)}\). The matrix \(H^{-1}KH^{-T}\) is still symmetric. However, one can notice that the preconditioned residual satisfies

\[
H^{-1}r^{(k)} = \|r^{(k)}\|_{P^{-1}}\text{ where} \quad \|\cdot\|_{P^{-1}} \text{ is the norm arising from the inner product induced by } P^{-1}, \text{ i.e.}, \langle \cdot, \cdot \rangle_{P^{-1}} = \langle P^{-1}, \cdot \rangle. \quad \text{One further notes that we have the equivalence}
\]

\[
K_j(H^{-1}KH^{-T},H^{-1}r^{(0)}) = H^{-1}K_j(KP^{-1},r^{(0)}).
\]

If preconditioned MINRES at iteration \(j\) produce a correction

\[
s^{(j)} \in K_j(H^{-1}KH^{-T},H^{-1}r^{(0)}) \quad \text{such that} \quad y^{(j)} = y^{(0)} + s^{(j)},
\]

then we recover the approximation for \(x\) with \(x^{(j)} = H^{-T}(y^{(0)} + s^{(j)})\). Since \(x^{(0)} = H^{-T}y^{(0)}\) the correction space for preconditioned MINRES with respect to the original variables is actually \(P^{-1}K_j(KP^{-1},r^{(0)})\). From here, one can show that the preconditioned MINRES iteration is equivalent to an iteration with the subspace \(K_j(KP^{-1},r^{(0)})\) but with respect to the inner product \(\langle \cdot, \cdot \rangle_{P^{-1}}\) induced by the preconditioner. This is indeed a short-term recurrence iteration, as it can be shown that \(KP^{-1}\) is symmetric with respect to \(\langle \cdot, \cdot \rangle_{P^{-1}}\). Thus the derivation of the preconditioned MINRES method [2, Algorithm 4.1] can be presented as a small modification of the unpreconditioned MINRES [2, Algorithm 2.4].

This same fact was also shown in [5] but by interpreting the underlying operator as a mapping from a Hilbert space to its dual. There are many benefits to this interpretation. One advantage is that even in the finite dimensional situation, it allows the derivation of preconditioned MINRES without the temporary introduction of Cholesky factors.

Let the columns of \(V_j\) still form an orthonormal basis for a Krylov subspace, but this time the space \(K_j(KP^{-1},r^{(0)})\), and the orthonormality is with respect to \(\langle \cdot, \cdot \rangle_{P^{-1}}\). Let \(Z_j = P^{-1}V_j\) have as columns the image of those vectors under the action of the preconditioner. Then we have the preconditioned Lanczos relation,

\[
KP^{-1}V_j = KZ_j = V_jT_j
\]

where \(T_j\) has the tridiagonal structure described earlier. What differs here is that the columns of \(V_j\) have been orthonormalized with respect to the \(P^{-1}\) inner product, and
the entries of the tridiagonal matrix $T_j$ are formed from these $P^{-1}$ inner products. We have the three-term recurrence

$$\tag{2.5} Kz_j = \gamma_{j+1}v_{j+1} + \delta_jv_j + \gamma_jv_{j-1}. $$

The preconditioned MINRES method solves the following residual minimization problem,

$$\tag{2.6} x^{(j)} = x^{(0)} + Z_j y^{(j)} \text{ where } y^{(j)} = \underset{y \in R^j}{\text{argmin}} \|\gamma_1 e_1 - T_j y\|_2, $$

where $\gamma_1 = \|r^0\|_{P^{-1}}$.

Though this reduces the minimization of the residual to a small least-squares problem, this is not the most efficient way to implement the MINRES method; and indeed, this is not what is done in, e.g., [2, Algorithm 4.1]. Due to (2.3), MINRES can be derived such that only six full-length vectors must be stored. In the interest of not again deriving everything, we will simply provide a few relationships between quantities from the above explanation of MINRES and those in [2, Algorithm 4.1]. Further implementation details can be found in, e.g., [4, Section 2.5].

Let $T_j = Q_j R_j$ be a QR-factorization of $T_j$ computed with Givens rotations where $Q_j \in R^{(j+1) \times (j+1)}$ is a unitary matrix constructed from the product of Givens rotations, and $R_j \in R^{(j+1) \times j}$ is upper triangular. The matrix $R_j \in R^{j \times j}$ is simply $R_j$ with the last row (of zeros) deleted. We can write the matrix $Q_j^T$ as the product of the Givens rotation used to triangularize $T_j$. Since $T_j$ is tridiagonal and Hessenberg, we must annihilate only one subdiagonal entry per column. Following from [2, Algorithm 4.1], we denote $s_i$ and $c_i$ to be the Givens sine and cosine used to annihilate the $i$th entry of column $i - 1$ using the unitary matrix $F_i = \begin{bmatrix} c_i & s_i \\ -s_i & c_i \end{bmatrix}$. Thus we can denote

$$Q_j^T = G_{j+1}^{(j)} G_j^{(j)} \cdots G_2^{(j)}$$

where we define $G_i^{(j)} \in R^{(j+1) \times (j+1)}$ to be the matrix applying the $i$th Givens rotation to rows $i - 1$ and $i$ to a $(j + 1) \times (j + 1)$ matrix. Using a normal equations formulation of (2.6), we can derive an expression for the least squares minimizer

$$y^{(j)} = R_j^{-1} \{Q_j^T (\gamma_1 e_1)\}_{1:j},$$

where $\{ \}_1:j$ indicates we take only the first $j$ rows of the argument. For the purpose of discussion, we make an additional modification to the variable naming using in [2, Algorithm 4.1]. We index $\eta_j$ which is used to track the residual norm. On Line 4 of the algorithm, we would have $\eta_0 = \gamma_1$, and at Line 18, we would write $\eta_j = -s_{j+1} \eta_{j-1}$. From the proof of [3, Corollary 2.5.3], one can see that at iteration $j$, the least squares residual can be written

$$\gamma_1 e_1 - T_j y^{(j)} = Q_j (\eta_j e_{j+1}),$$

where $e_{j+1}$ is the last column of the $(j + 1) \times (j + 1)$ identity matrix, and because $Q_j$ is unitary, it follows that $|\eta_j|$ is the norm of the residual $\|r^{(j)}\|_{P^{-1}}$ pertaining to $x^{(j)}$.

We now derive an expression for the norms of $r_u^{(j)}$ and $r_p^{(j)}$ in terms of quantities arising in the Lanczos process and residual minimization. Due to the block structure...
of K, we partition \( V_j \) and \( Z_j \) similarly,

\[
V_j = \begin{bmatrix} V_{j,u} \\ V_{j,p} \end{bmatrix} \quad \text{and} \quad Z_j = \begin{bmatrix} Z_{j,u} \\ Z_{j,p} \end{bmatrix}
\]

and then insert the partitioned vectors into \( (2.2) \)

\[
\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} Z_{j,u} \\ Z_{j,p} \end{bmatrix} = \begin{bmatrix} AZ_{j,u} + B^T Z_{j,p} \\ BZ_{j,u} - CZ_{j,p} \end{bmatrix} = \begin{bmatrix} V_{j+1,u} \\ V_{j+1,p} \end{bmatrix} T_j = \begin{bmatrix} V_{j+1,u} T_j \\ V_{j+1,p} T_j \end{bmatrix}.
\]

We note that for tracking and updating the full residual vector, this partition is artificially imposed. One could simply track the full residual and partition at the end to compute the subvector norms separately. We derive everything using this block partition because one may wish to track the norm of only one subvector. Furthermore, one needs the partition quantities to define the recursions for updating the preconditioned subvector norms. It then follows that we have Lanczos relations for the blocks

\[
AZ_{j,u} + B^T Z_{j,p} = V_{j+1,u} T_j \quad \text{and} \quad BZ_{j,u} - CZ_{j,p} = V_{j+1,p} T_j.
\]

From [3, Theorem 2.5.7], we know that the \( j \)th MINRES residual satisfies the recursion

\[
r^{(j)} = r^{(j-1)} - c_{j+1} \eta_j^{-1} m_j^{(j+1)},
\]

where the auxiliary vectors can also be progressively updated. The progressive updating scheme for the auxiliary vectors can also be seen by observing that these auxiliary vectors form an orthonormal basis for the constraint space \( K P^{-1} K_j (K P^{-1}, r^{(0)}) \), namely

\[
M_{j+1} = V_{j+1} Q_j = \begin{bmatrix} m_1^{(j+1)} & m_2^{(j+1)} & \cdots & m_j^{(j+1)} & m_{j+1}^{(j+1)} \end{bmatrix}.
\]

Using induction, one can show that since \( Q_j \) is the product of Givens rotations with \( Q_j = Q_{j-1} G_j^{(j+1)}, \) we have that \( m_i^{(j+1)} = m_i^{(j)} \) for all \( 1 \leq i \leq j - 1, \) and

\[
m_j^{(j+1)} = c_{j+1} m_j^{(j)} + s_{j+1} v_{j+1} \quad \text{and} \quad m_{j+1}^{(j+1)} = -s_{j+1} m_j^{(j)} + c_{j+1} v_{j+1},
\]

where we set \( m_1^{(1)} = v_1. \) This implies that we can drop the superindices for the first \( j - 1 \) columns of \( M_{j+1} \) which remain unchanged, i.e.,

\[
M_{j+1} = \begin{bmatrix} m_1 & m_2 & \cdots & m_{j-1} & m_j^{(j+1)} & m_{j+1}^{(j+1)} \end{bmatrix}.
\]

From \( (2.8), \) we then have that

\[
r^{(j)} = \eta_j V_{j+1} Q_j e_{j+1} = \eta_j m_{j+1}^{(j+1)}.
\]

If we then partition the vector \( m_{j+1}^{(j+1)} = \begin{bmatrix} m_{j+1,u}^{(j+1)} \\ m_{j+1,p}^{(j+1)} \end{bmatrix}, \) we then have formulas for the partial residuals,

\[
r_u^{(j)} = \eta_j m_{j+1,u}^{(j+1)} \quad \text{and} \quad r_p^{(j)} = \eta_j m_{j+1,p}^{(j+1)}.
\]
We can also rewrite (2.13) in order to recover (2.11). By direct computation with some substitutions, we see that

\[ r^{(j)} = \eta_j m^{(j+1)} = (-s_j+1\eta_j-1) \left( -s_j+1m_j^{(j)} + c_j+1v_j+1 \right) \]

\[ = s_j+1\eta_j-1m_j^{(j)} + c_j+1s_j+1\eta_j-1v_j+1 \]

\[ = \eta_j-1m_j^{(j)} - c_j+1\eta_j-1m_j^{(j)} + c_j+1s_j+1\eta_j-1v_j+1 \]

\[ = r^{(j-1)} - c_j+1 \left( c_j+1\eta_j-1m_j^{(j)} + s_j+1\eta_j-1v_j+1 \right) \]

\[ = r^{(j-1)} - c_j+1\eta_j-1m_j^{(j+1)}. \]

Thus the residual subvectors \( r_u^{(j)} \) and \( r_p^{(j)} \) satisfy the progressive updating formulas

\[ r_u^{(j)} = r_u^{(j-1)} - c_j+1\eta_j-1m_j^{(j+1)} \quad \text{and} \quad r_p^{(j)} = r_p^{(j-1)} - c_j+1\eta_j-1m_j^{(j+1)}. \]

However, this representation would require storage of two full-length vectors.

We have seen that through recursion formulas, we can compute one or both subvectors of the residual vector produced by preconditioned MINRES. However, we wish to avoid storing or re-evaluating these vectors since we actually want to compute only the appropriate norms of each piece. The full residual minimization is with respect to the \( P^{-1} \) norm \( \| \cdot \|_{P^{-1}} \). We have assumed in this paper that the preconditioner has block diagonal structure; and as \( P \) is symmetric positive definite, it follows that its blocks are as well. Thus we can write

\[ \| r^{(j)} \|_{P^{-1}}^2 = \| r_u^{(j)} \|_{P_u^{-1}}^2 + \| r_p^{(j)} \|_{P_p^{-1}}^2. \]

These norms can also be computed recursively using information already on hand. We note that doing it as in the following allows us to avoid additional applications of the preconditioner.

In order to compute the norms separately, it is necessary that we also use the same fact for the newest Lanczos vector,

\[ 1 = \| v_{j+1} \|_{P^{-1}}^2 = \| v_{j+1,u} \|_{P_u^{-1}}^2 + \| v_{j+1,p} \|_{P_p^{-1}}^2. \]

Let

\[ \psi_{j+1,u} = \| v_{j+1,u} \|_{P_u^{-1}}^2 = \langle z_{j+1,u}, v_{j+1,u} \rangle \quad \text{and} \quad \psi_{j+1,p} = \| v_{j+1,p} \|_{P_p^{-1}}^2 = \langle z_{j+1,p}, v_{j+1,p} \rangle. \]

We can store these values so they are available for later use. We further denote \( \eta_{j,u} = \| r_u^{(j)} \|_{P_u^{-1}} \) and \( \eta_{j,p} = \| r_p^{(j)} \|_{P_p^{-1}} \). This allows us to concisely state the following theorem.

**Theorem 2.1.** The ratio between the full preconditioned residual norm and the respective preconditioned residual subvector norms can be written progressively as follows:

\[ \left( \frac{\eta_{j,u}}{\eta_j} \right)^2 = \frac{\eta_{j-1,u}}{\eta_{j-1}} \quad \text{and} \quad \left( \frac{\eta_{j,p}}{\eta_j} \right)^2 = \frac{\eta_{j-1,p}}{\eta_{j-1}} \]

\[ = 2s_j+1 \left( c_j+1 \right)^2 \left( m_{j,u}^{(j)} \right)^T z_{j+1,u} + c_j+1\psi_{j+1,u} \quad \text{and} \quad \left( \frac{\eta_{j-1,p}}{\eta_{j-1}} \right)^2 = 2s_j+1 \left( c_j+1 \right)^2 \left( m_{j,p}^{(j)} \right)^T z_{j+1,p} + c_j+1\psi_{j+1,p}. \]
Proof. The proofs for each subvector are identical, so we prove it only for one. We can verify the identity by direct calculation and then by showing that the quantities arising from the calculation are available by recursion. We compute

\[
\|r_u^{(j)}\|_{P_u^{-1}}^2 = \eta_j (m_{j+1,u}^{(j+1)})^T P_u^{-1} (m_{j+1,u}) = \eta_j (s_{j+1} m_{j+1,u} + c_{j+1} v_{j+1,u})^T P_u^{-1} (-s_{j+1} m_{j+1,u} + c_{j+1} v_{j+1,u}) \\
= \eta_j^2 (s_{j+1} m_{j+1,u})^T P_u^{-1} m_{j+1,u} - 2s_{j+1} c_{j+1} (m_{j,u})^T P_u^{-1} v_{j+1,u} \\
+ c_{j+1}^2 v_{j+1,u}^T P_u^{-1} v_{j+1,u} \\
= \eta_j^2 (s_{j+1}^2 \eta_{j-1,u} - 2s_{j+1} c_{j+1} (m_{j,u})^T z_{j+1,u} + c_{j+1}^2 s_{j+1}^2 \eta_{j+1,u}),
\]

Basic algebra finishes the proof.

For completeness, we now present a modified version of [2, Algorithm 4.1], here called algorithm 1. Note that we omit superscripts for the calculation where they are not needed. Furthermore, we introduce the scalars \(\theta_u\) and \(\theta_p\) defined by

\[
(2.14) \quad \theta_u = \langle m_{j,u}, z_{j+1,u} \rangle \quad \text{and} \quad \theta_p = \langle m_{j,p}, z_{j+1,p} \rangle
\]

and the squared residual norm fractions

\[
(2.15) \quad \mu_u = \left( \frac{\eta_{j,u}}{\eta_j} \right)^2 \quad \text{and} \quad \mu_p = \left( \frac{\eta_{j,p}}{\eta_j} \right)^2.
\]

Notice that one can work with full-length vectors and the partitioning is only important for the computation of partial inner products as in (2.14).

3. Examples and Numerical Experiments. In the introduction, we motivated our study by mentioning that the residual subvectors in saddle-point systems (1.1) often have different physical interpretations. In this section, we discuss several examples to underline this fact, and we also present numerical results which demonstrate the correctness of algorithm 1. We do this by storing all the residual vectors throughout the iteration and evaluating the preconditioned subvector norms a-posteriori. This is a debugging step which is introduced to verify the correctness of algorithm 1. Our MATLAB implementation of algorithm 1 is available at [6].

In all examples, we begin with an all-zero initial guess and we stop when the relative reduction of the total residual

\[
\frac{\eta_j}{\eta_0} = \frac{\|r^{(j)}\|_{P^{-1}}}{\|r^{(0)}\|_{P^{-1}}}
\]

falls below \(10^{-6}\). We could easily utilize a refined stopping criterion such as

\[
|\eta_{j,u}| = \|r_{u}^{(j)}\|_{P^{-1}} \leq \varepsilon_u \quad \text{and} \quad |\eta_{j,p}| = \|r_{p}^{(j)}\|_{P^{-1}} \leq \varepsilon_p
\]

to take advantage of the ability to monitor the residual subvector norms. Concrete applications of this (e.g., in optimization) are outside the scope of this paper and will be addressed elsewhere.
Algorithm 1: The preconditioned MINRES method with monitoring of \(|\eta_{j,u}| = \|r_u^{(j)}\|_{P^{-1}}\) and \(|\eta_{j,p}| = \|r_p^{(j)}\|_{P^{-1}}\).

Input: \(K \in \mathbb{R}^{(m+p) \times (m+p)}\), symmetric, and \(f \in \mathbb{R}^{m+p}\) as in (1.1), \(P = \text{blkdiag}(P_u, P_p) \in \mathbb{R}^{(m+p) \times (m+p)}\), symmetric positive definite.

Output: \(x^{(j)}\) for some \(j\) such that \(\|r^{(j)}\|_{P^{-1}}\) satisfies some convergence criteria.

1. Set \(v_0 = 0\), \(w_0 = w_1 = 0\).
2. Choose \(x^{(0)}\), set \(v_1 = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} - Kx^{(0)}\), \(z_1 = P^{-1}v_1\).
3. \(\gamma_1 = \sqrt{(z_1, v_1)}, \ v_1 \leftarrow v_1 / \gamma_1, \ z_1 \leftarrow z_1 / \gamma_1\).
4. \(\psi_u = (z_{1,u}, v_{1,u}), \ \psi_p = (z_{1,p}, v_{1,p})\).
5. \(\mu_u = \psi_u, \ \mu_p = \psi_p\).
6. \(m_1 = v_1\).
7. Set \(\eta_0 = \gamma_1, \ \eta_{0,u} = \gamma_1 \sqrt{\psi_u}, \ \eta_{0,p} = \gamma_1 \sqrt{\psi_p}, \ s_0 = s_1 = 0, \ c_0 = c_1 = 1\).
8. for \(j = 1\) until convergence do
   \(\delta_j = (Kz_j, z_j)\).
   \(v_{j+1} = Kz_j - \delta_j v_j - \gamma_j v_{j-1}\) // Lanczos
   \(z_{j+1} = P^{-1} v_{j+1}\).
   \(v_{j+1} = \sqrt{(z_{j+1}, v_{j+1})}\).
   \(z_{j+1} = z_{j+1} / \gamma_{j+1}\).
   \(a_0 = c_j \delta_j - c_{j-1} s_j \gamma_j\) // Update QR factorization
   \(a_1 = \sqrt{a_0^2 + \gamma_j^2}\).
   \(a_2 = s_j \delta_j + c_{j-1} c_j \gamma_j\).
   \(a_3 = s_j \gamma_j - a_0 / a_1\) // Givens rotations
   \(\theta_u = z_{j,u} + s_j \delta_j, \ \theta_p = z_{j,p} - c_j \gamma_j\).
   \(\psi_u = (z_{j+1,u}, v_{j+1,u}), \ \psi_p = (z_{j+1,p}, v_{j+1,p})\).
   \(m_{j+1} = -(s_j + 1) m_j + c_j v_{j+1}\).
   \(w_{j+1} = z_j - a_3 w_{j-1} - a_2 w_j / a_1\).
   \(x^{(j)} = x^{(j-1)} + c_j z_{j-1} / \gamma_j + \theta_j - 1 w_{j+1}\).
   \(\mu_u = s_j \mu_u + 2 s_j + 1 c_j \gamma_j / \gamma_j + 1^2 \psi_u\).
   \(\mu_p = s_j \mu_p + 2 s_j + 1 c_j \gamma_p / \gamma_j + 1^2 \psi_p\).
   \(\eta_j = -s_j + \eta_j / \gamma_j - 1\) // total residual norm
   \(\eta_{j,u} = \eta_j \sqrt{\mu_u}, \ \eta_{j,p} = \eta_j \sqrt{\mu_p}\) // partial residual norms
9. Test for convergence.

Example 3.1 (Least-Norm Solution of Underdetermined Linear System).

We consider an underdetermined and consistent linear system \(Bu = b\) with a matrix \(B \in \mathbb{R}^{n \times m}\) of full row rank and \(m < n\). Its least-norm solution \(u^* \in \mathbb{R}^n\) in the sense of the inner product defined by the symmetric positive definite matrix

\[
\text{Minimize} \quad \frac{1}{2} \|u\|^2_H \quad \text{such that} \quad Bu = b, \quad u \in \mathbb{R}^n
\]
\( H \in \mathbb{R}^{n \times n} \), is uniquely determined by the saddle-point system
\[
\begin{bmatrix}
H & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
u \\
p
\end{bmatrix}
= \begin{bmatrix} 0 \\ b \end{bmatrix}.
\]

Notice that the first block of equations represents optimality, while the second block represents feasibility of a candidate solution \((u, p)^T\).

Our test case uses data created through the commands
\[
\text{rng}(42); \ n=100; \ m=30; \ B= \text{randn}(m,n); \ b= \text{randn}(m,1); \\
H= \text{spdiags}(\text{rand}(n,1),0,n,n);
\]
As preconditioner we use either \( P_1 = \text{blkdiag}(I_{n \times n}, I_{m \times m}) \) (the unpreconditioned case) or \( P_2 = \text{blkdiag}(H, I_{m \times m}) \). The convergence histories in Figure 3.1 show that the amount by which the two residual subvectors contribute to their combined norm may indeed be quite different, and it depends on the preconditioner. In this example, the feasibility residual \( r_p = b - Bu \) is significantly smaller than the optimality residual \( r_u = -Hu - B^T p \) in the unpreconditioned case where we used \( P_1 \). To be more precise, the average value of \( \mu_p \) throughout the iteration history is about 21%. Quite the opposite is true for the case of \( P_2 \), when \( \mu_p \) is close to 100%.

**Example 3.2 (Least-Squares Solution of Overdetermined Linear System).**
Here we consider an overdetermined linear system \( B^T p = b \) with a matrix \( B \in \mathbb{R}^{m \times n} \) of full row rank and \( m < n \). Its least-squares solution
\[
\text{Minimize} \quad \frac{1}{2} \| B^T p - b \|_{H^{-1}}, \quad p \in \mathbb{R}^m
\]
with \( H \in \mathbb{R}^{n \times n} \) symmetric positive definite as above, is uniquely determined by the normal equations, \( BH^{-1}(B^T p - b) = 0 \). By defining \( u \) as the 'preconditioned residual' \( H^{-1}(B^T p - b) \), we find that the least-squares solution is in turn equivalent to the saddle-point system
\[
\begin{bmatrix}
H & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
u \\
p
\end{bmatrix}
= \begin{bmatrix} b \\ 0 \end{bmatrix}.
\]
The first block of equations now represents feasibility for the constraint defining the auxiliary quantity \( \mathbf{u} \), while the second requires \( \mathbf{u} \) to lie in the kernel of \( B \).

Similarly as above, we derive test data through:

\[
\text{rng}(42); \quad n=100; \quad m=30; \quad B=\text{randn}(m,n); \quad b=\text{randn}(n,1);
\]

\[
H=\text{spdiags}(\text{rand}(n,1),0,n,n);
\]

We employ the same preconditioners \( \mathbf{P}_1 \) and \( \mathbf{P}_2 \) as in Example 3.1. Once again, the convergence behavior of the two residual subvectors is fundamentally different (Figure 3.2) for the two cases: in the unpreconditioned case, the average value of \( \mu_p \) is about 9\%, while it is 72\% in the preconditioned case.

Our remaining examples involve partial differential equations and they will be stated in variational form, by specifying bilinear forms \( a(\cdot,\cdot) : V \times V \to \mathbb{R} \), \( b(\cdot,\cdot) : V \times Q \to \mathbb{R} \), and, where appropriate, \( c(\cdot,\cdot) : Q \times Q \to \mathbb{R} \). Here \( V \) and \( Q \) are (real) Hilbert spaces. The matrices \( \mathbf{A} \), \( \mathbf{B} \) and \( \mathbf{C} \) in (1.1) are then obtained by evaluating the respective bilinear forms on a basis of an appropriate finite dimensional subspace \( V_h \) or \( Q_h \), e.g., \( [\mathbf{B}]_{ij} = b(\varphi_j, \psi_i) \) for basis elements \( \varphi_j \in V_h \) and \( \psi_i \in Q_h \). Similarly, the right hand side vectors \( \mathbf{f}_u \) and \( \mathbf{f}_p \) are obtained from evaluating problem dependent linear forms \( f_u(\cdot) \) and \( f_p(\cdot) \) on the same basis functions \( \varphi_i \) and \( \psi_i \), respectively. Finally, the matrices and vectors obtained in this way may need to be updated due to the incorporation of essential (Dirichlet) boundary conditions.

All numerical tests were conducted using the Python interface of the finite element library FEniCS [7] (version 1.6) to generate the matrices and vectors. Those were then exported in PETSc binary format and read from MATLAB through the helper functions readPetscBinMat.m and readPetscBinVec.m provided by Samar Khatiwala on his web page. We deliberately turned off the reordering feature of FEniCS for the degrees of freedom to preserve the block structure of (1.1) for illustration purposes (see Figure 3.6) and in order for the subvectors \( \mathbf{u} \) and \( \mathbf{p} \) and the residuals \( \mathbf{r}_u \) and \( \mathbf{r}_p \) to remain contiguous in memory. However, our theory does not rely on a particular ordering of the subvector components, and our implementation of algorithm 1 allows for arbitrary component ordering.

It will turn out to be useful for the following examples to specify the physical units (Newton: N, meters: m, seconds: s, Watt: W, and Kelvin: K) for all involved quantities in the following examples.
EXAMPLE 3.3 (Stokes Channel Flow).

We consider the variational formulation of a 3D stationary Stokes channel flow configuration within the domain \( \Omega = (0,10) \times (0,1) \times (0,1) \). Dirichlet conditions are imposed on the fluid velocity \( u \) everywhere except at the 'right' (outflow) boundary \( (x = 10) \), where do-nothing conditions hold. The Dirichlet conditions are homogeneous (no-slip) except at the 'left' (inflow) boundary \( (x = 0) \), where \( u(x,y,z) = u_\text{in}(x,y,z) = (y(1-y)z(1-z),0,0)^T \) m s\(^{-1}\) is imposed.

Appropriate function spaces for this setup are \( V = \{ v \in H^1(\Omega;\mathbb{R}^3) : v = 0 \text{ on } \Gamma \setminus \Gamma_{\text{right}} \} \) for the velocity and \( Q = L^2(\Omega) \) for the pressure. The relevant bilinear and linear forms associated with this problem are

\[
a(u,v) = \mu \int_\Omega \nabla u : \nabla v \, dx, \quad b(u,q) = \int_\Omega q \text{ div } u \, dx \quad \text{and} \quad f_u(v) = \int_\Omega f \cdot v \, dx.
\]

We use the dynamic viscosity parameter \( \mu = 1 \times 10^{-3} \text{Ns m}^{-2} \) (water) and zero right hand side force \( f = (0,0,0)^T \) N m\(^{-3}\).

By considering units, or by investigating the underlying physics, we infer that the first component of the residual, \( r_u = f_u - a(u,\cdot) - b(\cdot,p) \), represents a net sum of forces, measured in N. Similarly, the second residual \( r_p = -b(u,\cdot) \) represents the net flux of fluid through the impermeable channel walls, measured in m\(^3\) s\(^{-1}\). Clearly, both parts of the residual must be zero at the converged solution, but their departure from zero at intermediate iterates has different physical interpretations.

As preconditioner \( P = \text{blkdiag}(P_u, P_p) \), we use the block diagonal matrix induced by the bilinear forms

\[
a(u,v) \quad \text{and} \quad \mu^{-1} \int_\Omega pq \, dx,
\]

respectively, similar to \[2, \text{Section 4.2}\], where the constant-free problem is considered. Notice that the inclusion of the constant \( \mu^{-1} \) into the pressure mass matrix renders the preconditioner compatible with the physical units of the problem.

For our numerical test, we discretized the problem using the Taylor-Hood finite element. The homogeneous and non-homogeneous Dirichlet boundary conditions were included by modifying the saddle-point components \( A, B, B^T \), and right hand side \( f_u \) in (1.1) in a symmetric way through the \texttt{assemble_system} call in FEniCS. Notice that this effectively modifies some components of the first residual subvector \( r_u \) by expressions of the form \( u_\text{in}(x,y,z) - u(x,y,z) \), measured in ms\(^{-1}\). The same modifications apply to the preconditioner \( P \).

Figure 3.3 displays the convergence behavior of the residual subvector norms on a relatively coarse mesh and its refinement. The result illustrates the mesh independence of the preconditioned iteration, and it also shows that the residual \( r_p \) (representing mass conservation) lags behind the residual \( r_u \) over the majority of the iterations.

EXAMPLE 3.4 (Linear Elasticity with Nearly Incompressible Material).

This example describes a tensile test with a rod of square cross section, which occupies the domain \( \Omega = (0,100) \times (0,10) \times (0,10) \). We use mm here in place of m as our length unit. Homogeneous Dirichlet conditions for the displacement \( u \) are imposed at the 'left' (clamping) boundary \( (x = 0) \), while natural (traction) boundary conditions are imposed elsewhere. The imposed traction pressure is zero except at the 'right' (forcing) boundary \( (x = 100) \), where a uniform pressure of \( g = (1,0,0)^T \) N mm\(^{-2}\) is imposed. As is customary for nearly incompressible material, we introduce an extra

\[
\text{MONITORING OF RESIDUAL IN SADDLE-POINT PROBLEMS}
\]
variable $p$ for the hydrostatic pressure (see for instance [11]) in order to overcome the ill-conditioning of a purely displacement based formulation known as locking [1]. We employ the standard isotropic stress-strain relation, $\sigma = 2 \mu \varepsilon (u) + p I$ and $\text{div} \ u = \lambda^{-1} p$. Here $\varepsilon(u) = (\nabla u + \nabla u^T)/2$ denotes the symmetrized Jacobian of $u$, while $\mu$ and $\lambda$ denote the Lamé constants. We choose as material parameters Young’s modulus $E = 50 \text{N mm}^{-2}$ and a Poisson ratio of $\nu = 0.49$. These particular values describe a material like nearly incompressible rubber, and a conversion to the Lamé constants yields $\mu = \frac{E}{2(1+\nu)} = 16.78 \text{N mm}^{-2}$ and $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} = 822.15 \text{N mm}^{-2}$.

The variational mixed formulation obtained in this way is described by the spaces $V = \{ v \in H^1(\Omega; \mathbb{R}^3) : v = 0 \text{ on } \Gamma_{bc} \}$ for the displacement and $Q = L^2(\Omega)$ for the hydrostatic pressure. The bilinear and linear forms associated with this problem are

$$a(u, v) = 2 \mu \int_\Omega \varepsilon(u) : \varepsilon(v) \, dx,$$

$$b(u, q) = \int_\Omega q \, \text{div} \, u \, dx,$$

$$c(p, q) = \lambda^{-1} \int_\Omega pq \, dx \quad \text{and} \quad f_u(v) = \int_{\Gamma_{right}} g : v \, dx.$$

At the converged solution, the body is in equilibrium. At an intermediate iterate, we can interpret $r_u = f_u - a(u, \cdot) - b(\cdot, p)$ as a net force acting on the body, measured in N. This force is attributed to a violation of the equilibrium conditions $\text{div} \, \sigma = -f$ in $\Omega$, and $\sigma \, n = 0$ or $\sigma \, n = g$ at the non-clamping boundary parts at an intermediate iterate $(u, p)^T$. The second residual $r_p = -b(u, \cdot) + c(p, \cdot)$ admits an interpretation of a volume measured in $\text{m}^3$ due to a violation of $\text{div} \, u = \lambda^{-1} p$.

As preconditioner $P = \text{blkdiag}(P_u, P_p)$, we use the block diagonal matrix induced by the bilinear forms $a(u, v)$ and $c(p, q)$, respectively. Once again, we remark that this choice is compatible with the physical units of the problem.

Similarly as for Example 3.3, we discretize the problem using the Taylor-Hood finite element, and similar modifications due to Dirichlet displacement boundary conditions apply. Figure 3.4 illustrates the convergence behavior on successively refined meshes, revealing once again different orders of magnitude for the two components of the residual.

**Example 3.5 (Optimal Boundary Control).**

Our final example is an optimal boundary control problem for the stationary heat
The problem statement is

\[
\begin{align*}
\text{Minimize} & \quad \frac{\alpha_1}{2} \| u - u_d \|_{L^2(\Omega)}^2 + \frac{\alpha_2}{2} \| f \|_{L^2(\Gamma)}^2 \\
\text{s.t.} & \quad -\kappa \Delta u + \delta u = 0 \quad \text{in } \Omega, \\
& \quad \kappa \frac{\partial u}{\partial n} = f \quad \text{on } \Gamma.
\end{align*}
\]

As data we use \( \alpha_1 = 1 \, \text{m}^{-3} \, \text{K}^{-2} \), \( u_d(x,y,z) = x \, \text{K} \), \( \alpha_2 = 1 \times 10^{-2} \, \text{m}^2 \, \text{W}^{-2} \), heat conduction coefficient \( \kappa = 1 \, \text{W} \, \text{m}^{-1} \, \text{K}^{-1} \), and radiation coefficient \( \delta = 1 \, \text{W} \, \text{m}^{-3} \, \text{K}^{-1} \).

The necessary and sufficient optimality conditions for this problem are standard; see, for instance, [10, Chapter 2.8]. When we eliminate the control function \( f \) from the problem, a saddle-point system for the state \( u \) and adjoint state \( p \) remains, which is described by the following data:

\[
\begin{align*}
\alpha(u,v) &= \alpha_1 \int_{\Omega} u \, v \, dx, \quad b(u,q) = \kappa \int_{\Omega} \nabla u \cdot \nabla q \, dx + \delta \int_{\Omega} u \, q \, dx, \\
c(p,q) &= \alpha_2^{-1} \int_{\Gamma} p \, q \, ds \quad \text{and} \quad f_u(v) = \alpha_1 \int_{\Omega} u_d \, v \, dx.
\end{align*}
\]

The underlying spaces are \( V = Q = H^1(\Omega) \), and we discretize both using piecewise linear, continuous finite elements. Note that the elements \( u,v \in V \) are measured in \( \text{K} \) while the elements \( p,q \in Q \) are measured in \( \text{W}^{-1} \).

As preconditioner \( P = \text{hilbdiag}(P_u, P_p) \), we use the block diagonal matrix induced by the bilinear forms

\[
\begin{align*}
p_u(u,v) &= \alpha_1 \kappa \delta^{-1} \int_{\Omega} \nabla u \cdot \nabla v \, dx + \alpha_1 \int_{\Omega} u \, v \, dx, \\
p_p(p,q) &= \alpha_2^{-1}(\kappa \delta^{-1})^{1/2} \int_{\Omega} \nabla p \cdot \nabla q \, dx + \alpha_2^{-1}(\kappa^{-1} \delta)^{1/2} \int_{\Omega} p \, q \, dx,
\end{align*}
\]

respectively. As in our previous examples, this choice is compatible with the physical units of the problem. Figure 3.5 illustrates the convergence behavior on successively refined meshes. Besides the mesh independence, we observe that both residual subvector norms converge in unison in this example.
Fig. 3.5. Convergence history of the residual subvectors for Example 3.5 (optimal boundary control) on a coarse grid (left) and its uniform refinements (middle and right).

Fig. 3.6. Sparsity plots of the saddle-point systems arising in Example 3.1 (underdetermined linear system), Example 3.3 (Stokes), Example 3.4 (elasticity), and Example 3.5 (optimal boundary control).

4. Discussion. In this paper we developed a modified implementation of MINRES. When applied to saddle-point systems, the new implementation allows us to monitor the norms of the subvectors $\|r^{(j)}_u\|_{P^{-1}}$ and $\|r^{(j)}_p\|_{P^{-1}}$ individually, while conventional implementations keep track of only the total residual norm $\|r^{(j)}\|_{P^{-1}}$. It should be obvious how algorithm 1 generalizes to systems with more than two residual subvectors and block-diagonal preconditioners structured accordingly. The price to pay to monitor the subvector norms is the storage of one additional vector for components $m_{j,u}$ and $m_{j,p}$ compared to the implementation of MINRES given in [2, Algorithm 4.1] as well as some additional inner product calculations. It should be noted that if the cost of applying the operator and preconditioner are cheap enough, it may be preferable to simply construct the full residual and calculate preconditioned...
subvector norms explicitly. However, in the case that application of these operators has significant costs (particularly in the case that they are available only as procedures and never actually constructed) the method presented in this paper has important advantages.

While we developed the details in finite dimensions using matrices and vectors, our approach directly transfers to linear saddle-point systems in a Hilbert space setting using linear operators and linear forms, as described in [5].

Being able to differentiate between the contributions to the total residual offers new opportunities for the design of iterative algorithms for nonlinear problems, which require inexact solves of (1.1) as their main ingredient. We envision for instance solvers for equality constrained nonlinear optimization problems which may now assign individual stopping criteria for the residuals representing optimality and feasibility, respectively. The design of such an algorithm is, however, beyond the scope of this work. Similarly, for the Stokes Example 3.3, the user may now assign individual stopping criteria for the fulfillment of the balance of forces (first residual) and the conservation of mass (second residual).

A topic of future research could be to study the decay properties of the subvector norms, rather than study the decay of the total residual norm; see for instance [2, Section 4.2.4]. We expect that such an analysis will be more involved but it may shed light on how the relative scaling of the preconditioners blocks affects the convergence of the residual subvectors.

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