Symmetric inner-iteration preconditioning
for rank-deficient least squares problems

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April 6, 2015

Abstract
Stationary iterative methods with a symmetric splitting matrix are performed as inner-
iteration preconditioning for Krylov subspace methods. We give a necessary and sufficient
condition such that the inner-iteration preconditioning matrix is definite, and show that
conjugate gradient (CG) method preconditioned by the inner iterations determines a so-
lution of symmetric and positive semidefinite linear systems, and the minimal residual (MR)
method preconditioned by the inner iterations determines a solution of symmetric linear
systems including the singular case. These results are applied to the CG and MR-type
methods such as the CGLS, LSMR, and CGNE methods preconditioned by inner itera-
tions, and thus justify using these methods for solving least squares and minimum-norm
solution problems whose coefficient matrices are not necessarily of full rank. Thus, we
complement the theory of these methods presented in [K. Morikuni and K. Hayami, SIAM
J. Matrix Appl. Anal., 34 (2013), pp. 1–22], [K. Morikuni and K. Hayami, SIAM J. Matrix
Appl. Anal., 36 (2015), pp. 225–250], and give bounds for these methods.

Keywords: Rank-deficient least squares problems, Preconditioning, Krylov subspace
methods, Symmetric singular linear systems.

AMS subject classifications: 65F08, 65F10, 65F20, 65F50.

1 Introduction.
First, consider solving symmetric linear systems of equation

\[ Ax = b, \] (1.1)

where \( A = A^T \in \mathbb{R}^{n \times n} \) is not necessarily nonsingular and \( b \) is in the range space of \( A, \mathcal{R}(A) \).

In the symmetric and positive definite (SPD) case, i.e., \( v^T A v > 0 \) for all \( v \neq 0 \), the
conjugate gradient (CG) method [23] has been used. In the symmetric and positive semidefinite
(SPSD) case, i.e., \( v^T A v \geq 0 \) for all \( v \in \mathbb{R}^n \), for \( b \in \mathcal{R}(A) \), CG with the initial iterate
\( x_0 \in \mathbb{R}^n \) determines the \( k \)th iterate \( x_k \in x_0 + \mathcal{K}_k(A, r_0) \) that minimizes the A-seminorm
\( \|e_k\|_A = \|x_k - x_*\|_A \), where \( r_0 = b - Ax_0 \), \( \mathcal{K}_k(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\} \) is the
Krylov subspace of order \( k \), \( \|e\|_A = \sqrt{(e, e)_A} = \sqrt{(Ae, e)} \) is the semi inner product associated
with \( A \) SPSD, and

\[ x_* = A^#b + (I - A^#A)x_0, \] (1.2)
\(A^\#\) is the group inverse of \(A\), which satisfies

\[
AA^\# = A^\# A, \quad A^\# AA^\# = A^\#, \quad \begin{cases} AA^\# = I & \text{if } A \text{ is nonsingular}, \\ A^2A^\# = A & \text{if } A \text{ is singular}, \end{cases}
\]

(see [41, Theorem 3.2]), and \(I\) is the identity matrix. Note that since \(\text{index}(A) \leq 1\) from \(A = A^T\), \(A^\#\) is equal to the Drazin inverse of \(A\), where \(\text{index}(A) = \min\{d \in \mathbb{N}_0 \mid \text{rank} A^d = \text{rank} A^{d+1}\}\) and \(A^0 = I\). CG determines the solution \(x_\ast\) of (1.1) for all \(b \in \mathcal{R}(A)\) and for all \(x_0 \in \mathbb{R}^n\), and determines the minimum-norm solution \(A^\# b\) of (1.1) for all \(b \in \mathcal{R}(A)\) and for all \(x_0 \in \mathcal{R}(A)\). See [26], [20]. An error bound of CG is given by \(\|e_k\|_A \leq 2[(\sqrt{\kappa_2(A)} - 1)/(\sqrt{\kappa_2(A)} + 1)]^k\|e_0\|_A\), e.g., [27], where \(\kappa_2(A) = \|A\|_2\|A^{-1}\|_2\). Hence, the convergence is expected to be fast as \(\kappa_2(A)\) is small.

In the indefinite case, the minimal residual (MR) method has been used. Particular implementations of MR were presented in [39], [34], [13]. For \(b \in \mathbb{R}^n\), MR with \(x_0 \in \mathbb{R}^n\) determines the \(k\)th iterate \(x_k = x_0 + K_k(A, r_0)\) that minimizes \(\|r_k\|_2\). MR determines a solution of least squares problems \(\min_{x \in \mathbb{R}^n} \|b - Ax\|_2\) for all \(b \in \mathbb{R}\) and for all \(x_0 \in \mathbb{R}^n\), determines the solution of the form (1.2) for all \(b \in \mathcal{R}(A)\) and for all \(x_0 \in \mathbb{R}^n\), and determines the minimum-norm solution of (1.1) for all \(b \in \mathcal{R}(A)\) and for all \(x_0 \in \mathcal{R}(A)\). These arguments are given by the symmetric case of the generalized minimal residual method [6], [19]. Similarly, a residual bound of MR is given by \(\|r_k\|_2 \leq \varepsilon^k\|r_0\|_2\) with \(\varepsilon^k = \min_{p \in \mathbb{P}_k} \max_{\lambda \in \sigma(A)} |p(\lambda)|\), where \(\mathbb{P}_k\) is the set of all polynomials of degree not exceeding \(k\) and \(\sigma(A)\) is the spectrum of \(A\) [4, Theorem 1]. See [17], [23], [39], [34], [40], [42], [13] for other Krylov subspace methods for symmetric linear systems.

For accelerating the convergence of CG and MR, consider using preconditioning. See [25] for the preconditioned CG method in the singular case. Several steps of stationary iterative methods serve as preconditioning for Krylov subspace methods, which may be considered as inner iterations [30]. We consider using stationary iterative methods with a symmetric splitting matrix as inner-iteration preconditioning for CG and MR. To show that these methods determine a solution of symmetric and indefinite linear systems including the singular case, we give a necessary and sufficient condition such that the inner-iteration preconditioning matrix is definite and bounds for these methods. The condition is satisfied by using the Richardson, Jacobi overrelaxation (JOR), and symmetric successive overrelaxation (SSOR) methods [35], [24], [38] whose relaxation parameters are within certain intervals. Thus, we improve the theories in the SPD case [12], [1] for a general symmetric case. Also, inner-iteration preconditioning is a tractable extension of the splitting preconditioning [36, Section 10.2], which can be regarded as one step application of the inner iterations.

These methods have a potential to determine a solution of the normal equations

\[A^T A x = A^T b,\] (1.3)
equivalently least squares problems

\[
\min_{x \in \mathbb{R}^n} \|b - Ax\|_2, \quad (1.4)
\]

where \(A \in \mathbb{R}^{m \times n}\) is not necessarily of full rank and \(b \in \mathbb{R}^m\) is not necessarily in \(\mathcal{R}(A)\), using efficient implementations such as the CGLS, LSQR, and LSMR methods [23], [33], [16].

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The normal equations (1.3) form an SPSD linear system. For solving (1.4), the (preconditioned) CGLS and LSQR methods have been used, which both are mathematically equivalent to (preconditioned) CG applied to (1.3). Another option for solving (1.4) is to use the (preconditioned) LSMR method [16], which is mathematically equivalent to (preconditioned) MR applied to (1.3).

On the other hand, consider solving minimum-norm solution problems

$$\min \|x\|_2, \quad \text{subject to} \quad Ax = b, \quad b \in \mathcal{R}(A).$$  \hspace{1cm} (1.5)

The solution of (1.5) is the pseudo-inverse solution of $Ax = b, \quad b \in \mathcal{R}(A)$. The problem (1.5) is equivalent to the normal equations of the second kind

$$x = A^T u, \quad \text{subject to} \quad AA^T u = b, \quad b \in \mathcal{R}(A).$$  \hspace{1cm} (1.6)

Note that the constraint of (1.6) is an SPSD linear system. For solving (1.5), the (preconditioned) CGNE method [10] has been used, which is mathematically equivalent to (preconditioned) CG applied to the constraint of (1.6). Another option for solving (1.5) is to use the (preconditioned) MRNE method [31], which is mathematically equivalent to (preconditioned) MR applied to the constraint of (1.6).

We apply the above mentioned result for symmetric linear systems to CGLS, LSQR, LSMR, CGNE, and MRNE preconditioned by inner iterations, and thus justify using these methods particularly for rank-deficient least squares problems. CGLS and CGNE preconditioned by one step of SSOR-type methods were proposed in [5]. These methods were generalized to multistep versions in [30], [31]. In this paper, we complement the theory for the inner-iteration preconditioning for the CG and MR-type methods including the rank-deficient case. These methods have an advantage concerning memory requirement compared to the right- and left-preconditioned generalized minimal residual methods for least squares problems [21], [30], [31]. Numerical experiment results of these methods preconditioned by JOR and SSOR-type inner iterations were given in [31], [30].

The rest of the paper is organized as follows. In Section 2, we give conditions such that CG and MR preconditioned by inner iterations determine a solution of linear systems, and give bounds of these methods and conditions for specific stationary iterative methods that satisfy the condition. In Sections 3 and 4, we apply these results to CGLS, LSQR, and LSMR preconditioned by inner iterations for solving least squares problems and CGNE and MRNE preconditioned by inner iterations for solving minimum-norm solution problems, respectively. In Section 5, we conclude the paper.

## 2 Preconditioning for symmetric linear systems.

Consider solving symmetric linear systems (1.1). Let $P = P^T$ be a preconditioning matrix for (1.1). If $P$ is SPD, then the linear system (1.1) is equivalent to the preconditioned one $P^{-1}Ax = P^{-1}b$, or

$$P^{-\frac{1}{2}}AP^{-\frac{1}{2}}y = P^{-\frac{1}{2}}b, \quad x = P^{-\frac{1}{2}}y$$  \hspace{1cm} (2.1)

for all $b \in \mathcal{R}(A)$, where $P^{\frac{1}{2}}$ is the square root of $P$. If $\hat{A} = P^{-\frac{1}{2}}AP^{-\frac{1}{2}}, \hat{x} = P^{\frac{1}{2}}x$, and $\hat{b} = P^{-\frac{1}{2}}b$, (2.1) becomes $\hat{A}\hat{x} = \hat{b}$. For $b \in \mathcal{R}(A)$, CG applied to (2.1) (PCG) determines
$x_k = x_0 + \mathcal{K}_k(P^{-1}A, P^{-1}r_0)$ that minimizes $\|\tilde{e}_k\|_A$, equivalently CG applied to $P^{-1}Ax = P^{-1}b$ with the $P$-inner product does this, where $\hat{x}_k = x_k - \tilde{x}_k$.

$$\hat{x}_k = P^{-\frac{1}{2}}A^\#b + P^{-\frac{1}{2}}(I - A^\#A)\tilde{x}_0$$

(cf. (2.2)). For $b \in \mathcal{R}(A)$, MR applied to (2.1) (PMR) determines $x_k = x_0 + \mathcal{K}_k(P^{-1}A, P^{-1}r_0)$ that minimizes $\|\tilde{r}_k\|_2$, equivalently MR applied to $P^{-1}Ax = P^{-1}b$ with the $P$-inner product does this, where $\tilde{r}_k = b - \tilde{A}\hat{x}_k$. On the other hand, if $P$ is symmetric and negative definite (SND), i.e., $v^TAv < 0$ for all $v \neq 0$, then the linear system $Ax = b$ is equivalent to the preconditioned one $(-P)^{-1}Ax = (-P)^{-1}b$, or $(-P)^{-\frac{1}{2}}A(-P)^{-\frac{1}{2}}y = (-P)^{-\frac{1}{2}}b$, $x = (-P)^{-\frac{1}{2}}y$ for all $b \in \mathcal{R}(A)$. Without loss of generality, we restrict ourselves to the case where the preconditioning matrix is SPD for simplicity hereafter. Even when the preconditioning matrix is SND, the arguments below hold by changing the sign. Thus, we obtain the following.

**Lemma 2.1.** Assume that $A$ is SPSD and $P$ is SPD. Then, PCG determines a solution of $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathbb{R}^n$. The solution is of the form (2.2).

**Lemma 2.2.** Assume that $A = A^T$ and $P$ is SPD. Then, PMR determines a solution of $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathbb{R}^n$. The solution is of the form (2.2).

We note that PCG and PMR do not necessarily determine the minimum-norm solution $A^\#b$. Under the assumptions in Lemmas 2.1 and 2.2, PCG and PMR respectively determine the weighted minimum-norm solution $\arg\min ||P^{-\frac{1}{2}}x||_2$, subject to $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathcal{R}(P^{-1}A)$.

### 2.1 Inner-iterations preconditioned methods.

Consider using $\ell$ steps of a stationary iterative method as inner-iteration preconditioning for CG for SPSD linear systems. Let $C^{(\ell)}$ be the preconditioning matrix of $\ell$ inner iterations. An algorithm of this method is given as follows [3] (see [14] for efficient implementations).

**Algorithm 2.1.** CG method preconditioned by $\ell$ inner iterations

1. Let $x_0 \in \mathbb{R}^n$ be the initial iterate and $r_0 = b - Ax_0$.
2. Apply $\ell$ steps of a stationary iterative method to $Az = r_0$ to obtain $z_0 = p_0 = C^{(\ell)}r_0$.
3. For $k = 0, 1, 2, \ldots$ until convergence, Do.
4. $\alpha_k = (r_k, z_k)/(Ap_k, p_k)$, $x_{k+1} = x_k + \alpha_k p_k$, $r_{k+1} = r_k - \alpha_k Ap_k$
5. Apply $\ell$ steps of a stationary iterative method to $Az = r_{k+1}$ to obtain $z_{k+1} = C^{(\ell)}r_{k+1}$.
6. $\beta_k = (r_{k+1}, z_{k+1})/(r_k, z_k)$, $p_{k+1} = z_{k+1} + \beta_k p_k$
7. EndDo

We give an expression for the preconditioned matrix for CG with $\ell$ inner iterations. Consider the stationary iterative method applied to $Ax = r_k$ in lines 1 and 5. We call $A = M - N$ a splitting of $A$ and assume that $M$ is nonsingular. Denote the iteration matrix by $H = M^{-1}N$. Assume that the initial iterate is $z^{(0)} \in \mathcal{N}(H)$, e.g., $z^{(0)} = 0$. Then, the $\ell$th iterate of the stationary iterative method is $z^{(\ell)} = Hz^{(\ell-1)} + M^{-1}r_k = \sum_{i=0}^{\ell-1}H^iM^{-1}r_k$, $\ell \in \mathbb{N}$. Hence, the inner-iteration preconditioning matrix is $C^{(\ell)} = \sum_{i=0}^{\ell-1}H^iM^{-1}$. Therefore, the preconditioned matrix is $C^{(\ell)}A = \sum_{i=0}^{\ell-1}H^i(I - H) = I - H^\ell$. Conditions such that $C^{(\ell)}$ is definite will be given in Section 2.2. Under the conditions, one can set $P^{-1} = C^{(\ell)}$ and the arguments in
Lemma 2.1 follow. The inner-iteration preconditioning can be considered as the polynomial preconditioning using the truncated Neuman series expansion of $M^{-1}A$ [9] (see also [12], [14], [32], [2], [7], [15], [8], [29] and references therein).

On the other hand, consider the case of MR. Its algorithm is given as follows (cf. [14]).

Algorithm 2.2. MINRES method preconditioned by $\ell$ inner iterations

1. Let $x_0 \in \mathbb{R}^n$ be the initial iterate and $r_0 = b - Ax_0$
2. Apply $\ell$ steps of a stationary iterative method to $Ax = r_0$ to obtain $z_0 = C^{(\ell)}r_0$.
3. $\beta_0 = (r_0, z_0)^{1/2}$, $v_1 = r_0/\beta$, $u_1 = z_0/\beta$, $g_1 = 1$, $c_{-1} = 1$,
   $s_{-1} = 0$, $c_0 = 1$, $s_0 = 0$
4. For $k = 1, 2, \ldots$ until convergence, Do.
   5. $w = Au_k - \beta_{k-1}v_{k-1}$, $\alpha = (w, u_k)$, $w_k = w - \alpha_k v_k$
   6. Apply $\ell$ steps of a stationary iterative method to $Az = w_k$ to obtain $z_{k+1} = C^{(\ell)}w_k$.
   7. $\beta_k = (w_k, z_{k+1})^{1/2}$, $v_{k+1} = w_k/\beta_k$, $u_{k+1} = z_{k+1}/\beta_k$
   8. $\epsilon_k = s_{k-2}\beta_{k-1}$, $\delta_k = c_k - 2c_k\beta_{k-1} + s_{k-1}\alpha_k$
   9. $\gamma_k = -c_k - 2s_{k-1}\beta_{k-1} + c_{k-1}\alpha_k$, $\rho_k = (\beta_k^2 + \gamma_k^2)^{1/2}$
   10. $c_k = \gamma_k/\rho_k$, $s_k = \delta_k/\rho_k$, $\gamma_k = c_k\gamma_k$, $g_k = c_kg_k$, $g_{k+1} = -s_kg_k$
   11. $s_{k-1} = (u_k - \delta_k s_{k-2} - \epsilon_k s_{k-3})$, $d_{k-1} = \beta g_k$, $x_k = x_{k-1} + d_{k-1}s_{k-1}$
12. EndDo

The stationary iterative method applied to $Az = r_0$ and $Az = w_k$ in lines 2 and 5, respectively, gives the same preconditioning and preconditioned matrices as those in Algorithm 2.1. Polynomial preconditioning for indefinite Hermitian systems is presented in [18].

2.2 Definiteness of inner-iteration preconditioning matrices.

In order to examine the definiteness of the inner-iteration preconditioning matrix $C^{(\ell)}$, we extend [1, Lemma 1 and Theorem 1] to the general symmetric case $A = A^T$. We denote $A \sim B$ if $A$ and $B$ are similar and $A \equiv B$ if $A$ and $B$ are congruent.

Lemma 2.3. Assume that $A$ is SPD and $AB$ is symmetric. Then, the eigenvalues of $B$ are positive (negative) if and only if $AB$ is positive (negative) definite.

Proof. The lemma follows from $AB \sim A^{1/2}BA^{1/2} \equiv B$. □

Lemma 2.4. Assume that $AB$ is symmetric and $B$ is SPD. Then, the eigenvalues of $A$ are positive (negative) if and only if $AB$ is positive (negative) definite.

Proof. The lemma follows from $AB \sim B^{1/2}AB^{1/2} \equiv B$. □

Lemma 2.5. If $A$ is symmetric and definite (SD), i.e., either SPD or SND, and $B = B^T$, then $\sigma(AB) \subset \mathbb{R}$.

Proof. Assume that $A$ is SPD. Then, we have $\sigma(A^{1/2}BA^{-1/2}) \subset \mathbb{R}$, since it is symmetric. Hence, the eigenvalues of $AB \sim A^{1/2}BA^{1/2} \equiv B$ are real. On the other hand, assume that $A$ is SND. Since $-A$ is SPD, $\sigma([-A][-B]) \subset \mathbb{R}$. □

Lemma 2.6. If $A = A^T$ and $B$ is SD, then $\sigma(AB) \subset \mathbb{R}$.
Proof. Since the eigenvalues of \((AB)^T = B^TA^T\) are real from Lemma 2.5, we have \(\sigma(AB) \subseteq \mathbb{R} \). □

**Lemma 2.7.** If \(\ell \in \mathbb{N}\) and \(\sigma(A) \subseteq \mathbb{R}\), then the eigenvalues of \(\sum_{i=0}^{\ell-1} A^i\) are positive for all \(\ell\) odd.

**Proof.** If \(\lambda\) is an eigenvalue of \(A\) not equal to 1, then the corresponding eigenvalue of \(\sum_{i=0}^{\ell-1} A^i\) is \((1-\lambda^\ell)/(1-\lambda) > 0\). If \(\lambda = 1\), then the corresponding eigenvalue of \(\sum_{i=0}^{\ell-1} A^i\) is \(\ell > 0\). Hence, the eigenvalues of \(\sum_{i=0}^{\ell-1} A^i\) are positive for all \(\ell\) odd. □

Now we show the main theorem and give a necessary and sufficient condition such that the inner-iteration preconditioning matrix is SD.

**Theorem 2.8** (cf. [1, Theorem 1]). Let \(A = A^T\) be not necessarily nonsingular, \(\ell \in \mathbb{N}\), \(M = M^T\), \(N = M^{-1}N\), \(H = M^{-1}C\), \(C^{(\ell)} = \sum_{i=0}^{\ell-1} H^iM^{-1}\) be defined above. Then, the following hold.

1. \(C^{(\ell)}\) is symmetric.

2. For \(\ell\) odd, \(C^{(\ell)}\) is positive (negative) definite if and only if \(M\) is positive (negative) definite.

3. for \(\ell\) even, \(C^{(\ell)}\) is positive (negative) definite if and only if \(M + N\) is positive (negative) definite.

**Proof for 1.** Since \(N = N^T\), \(M^{-1}NM^{-1}N \cdots M^{-1}\) is symmetric. Hence, \(C^{(\ell)}\) is symmetric. □

**Proof for 2.** Assume that \(M\) is SPD (SND). Then, from Lemma 2.5, the eigenvalues of \(H = M^{-1}(M - A)\) are real. Since \(M^{-1}\) is SPD (SND), noting Lemma 2.7, \(C^{(\ell)} = \sum_{i=0}^{\ell-1} H^iM^{-1} = (-\sum_{i=0}^{\ell-1} H^i)(-M^{-1})\) is SPD (SND).

On the other hand, assume that \(C^{(\ell)}\) is SPD (SND). Then, the eigenvalues of \(\sum_{i=0}^{\ell-1} H^i = C^{(\ell)}M\) are real from Lemma 2.5, and positive from Lemma 2.7. Hence, from Lemma 2.3, \(M = (C^{(\ell)})^{-1}\sum_{i=0}^{\ell-1} H^i = (-C^{(\ell)})^{-1}(-\sum_{i=0}^{\ell-1} H^i)\) is positive (negative) definite. □

**Proof for 3.** Since \(\ell\) is even, we have

\[
MC^{(\ell)}M = M + MH + MH^2 + MH^3 + \cdots + MH^{\ell-1} = (M + N)(I + H^2 + H^4 + \cdots + H^{\ell-2}). \tag{2.3}
\]

Assume that \(M + N\) is SPD (SND). Since \(G = \sum_{i=0}^{(\ell-2)/2}(H^2)^i = (M + N)^{-1}MC^{(\ell)}M\), we have \(\sigma(G) \subseteq \mathbb{R}\) from Lemma 2.5, and \(\lambda > 0\) for all \(\lambda \in \sigma(G)\) from Lemma 2.7. Hence, \(MC^{(\ell)}M = (M + N)G = -(M + N)(-G) \equiv C^{(\ell)}\) is positive (negative) definite.

On the other hand, assume that \(C^{(\ell)} \equiv MC^{(\ell)}M\) is SPD (SND). Then, from (2.3), \(M + N\) is nonsingular. Since \((M + N)^{-1}\) is symmetric, the eigenvalues of \(G = (M + N)^{-1}MC^{(\ell)}M\) are real from Lemma 2.6, and positive from Lemma 2.7. Hence, \(M + N = MC^{(\ell)}MG^{-1} = (-MC^{(\ell)}M)(-G^{-1})\) is positive (negative) definite from Lemma 2.4. □

Letting \(A\) be positive definite in Theorem 2.8, we obtain [1, Theorem 1] as a corollary.
2.3 Convergence conditions.

We give sufficient conditions such that CG and MR preconditioned by inner iterations determine a solution of symmetric linear systems.

**Theorem 2.9.** Assume that $A = A^T$ is not necessarily nonsingular and $M = M^T$ is nonsingular such that $A = M - N$. Then, CG preconditioned by $\ell$ steps of the inner iterations $C^{(\ell)}$ defined above with $M$ definite for $\ell$ odd and $M + N$ definite for $\ell$ even, determines a solution of $Ax = b$ with $A$ SPSD for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathbb{R}^n$.

**Proof.** From Theorem 2.8, $C^{(\ell)}$ is SD for all $\ell \in \mathbb{N}$. Theorem 2.1 applied to CG for $C^{(\ell)}A^T x = C^{(\ell)}b$ with the $C^{(\ell)-1}$ inner product gives the theorem. □

**Theorem 2.10.** Under the same assumption in Theorem 2.9, MR preconditioned by $\ell$ steps of the inner iterations $C^{(\ell)}$ defined above with $M$ definite for $\ell$ odd and $M + N$ definite for $\ell$ even, determines a solution of $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathbb{R}^n$.

**Proof.** From Theorem 2.8, $C^{(\ell)}$ is SD for all $\ell \in \mathbb{N}$. Theorem 2.2 applied to MR for $C^{(\ell)}A^T x = C^{(\ell)}b$ the $C^{(\ell)-1}$ inner product gives the theorem. □

The solutions determined by these methods are given similarly to (2.2) with $P^{-1} = C^{(\ell)}$.

Theorems 2.9 and 2.10 will be applied to CG and MR-type methods for least squares and minimum-norm solution problems in Sections 3 and 4.

We note a relationship among definiteness, P-regularity, and semiconvergence. For a square matrix $A$, we say the splitting $A = M - N$ is P-regular if $M$ is nonsingular and $M + N$ is positive definite, i.e., the symmetric part of $M + N$ is SPD. Let $A = M - N$ be P-regular for $A$ symmetric, equivalently $M + M^T - A$ positive definite. Note that if $M = M^T$, then $M + M^T - A = 2M - A = M + N$. Then, $H = M^{-1}N$ is semiconvergent, i.e., $\lim_{i \to \infty} H^i$ exists, if and only if $A$ is positive semidefinite [28, Theorem 2]. Hence, for $A$ indefinite, $H = M^{-1}N$ is not semiconvergent even if $A = M - N$ is P-regular. Therefore, from Theorem 2.10, MR preconditioned by the inner iterations can determine a solution of $Ax = b$ even if $H$ is not semiconvergent, i.e., divergent. For example, if $A = \text{diag}(1, -1) = M - N$, $M = I$, and $N = \text{diag}(0, 2)$, then $M$ and $M + N$ are SPD but $H = M^{-1}N = N$ is divergent.

2.4 Convergence bounds.

Consider convergence bounds of CG and MR preconditioned by inner iterations. For the definiteness of the preconditioning matrix, assume that $C^{(\ell)}$ is SPD, or $M$ and $M + N$ are definite for $\ell$ both odd and even from Theorem 2.8.

First, we focus on CG. Assume that $A$ is SPSD or symmetric and negative semidefinite (SNSD), i.e., $v^TAv \leq 0$ for all $v \in \mathbb{R}^n$, and let $H = M^{-1}N$. From the proof of Theorem 2.8, we have $\sigma(H) \subset \mathbb{R}$. Denote the pseudo spectral radius of $H$ by $\nu(H) = \max\{|\lambda| : \lambda \in \sigma(H) \setminus \{1\}\}$ and the largest and smallest eigenvalues of $H$ not equal to 1 by $\lambda_{\text{max}}(H)$ and $\lambda_{\text{min}}(H)$, respectively. Since $H$ is semiconvergent [28, Theorem 2], equivalently $\nu(H) < 1$ and the eigenvalues of $H$ equal to 1 are simple [22], we have

$$
\kappa_2(C^{(\ell)}A) = \begin{cases} 
\frac{1 - \lambda_{\text{max}}(H)}{1 - \lambda_{\text{min}}(H)} & \text{for } \ell \text{ odd}, \\
\frac{(1 - \delta^\ell)/(1 - \nu(H)^\ell)}{1 - \nu(H)^\ell} & \text{for } \ell \text{ even},
\end{cases}
$$
where $\delta$ is the eigenvalue with the smallest absolute value of $H$. If $\kappa(\ell) = \kappa_2(C^{(\ell)}A)$, then an error bound of CG preconditioned by $\ell$ inner iterations is given as $\|e_k\|_A \leq 2(1/(\sqrt{\kappa(\ell)} + 1))^{k}\|e_0\|_A$. Thus, similar arguments in [1, Section 2.2] can be applied to the present SPSD (SNSD) case, defining the smallest eigenvalue of the iteration matrix by $\lambda_r$. In order to avoid repetition, we omit the detail.

On the other hand, we give a bound of MR preconditioned by $\ell$ inner iterations.

**Theorem 2.11.** If $A$ is SPSD and $H$ is semiconvergent, then the $k$th residual $r_k$ of MR preconditioned by $\ell$ steps of the inner iterations define above satisfies

$$\|\tilde{r}_k\|_2 \leq \min \left[ \nu(H)^{k\ell}, 2 \left( \frac{\sqrt{\kappa(\ell)} - 1}{\sqrt{\kappa(\ell)} + 1} \right)^k \right] \|\tilde{r}_0\|_2$$

(2.4)

for all $b \in R(A)$ and for all $x_0 \in \mathbb{R}^n$, where $\tilde{r}_k = C^{(\ell)} \tilde{r}_k$.

**Proof.** Theorem 2.10 ensures that MR preconditioned by the $\ell$ steps of the inner iterations determines a solution of $Ax = b$ for all $b \in R(A)$ and for all $x_0 \in \mathbb{R}^n$. From [4, Theorem 1], we have

$$\|\tilde{r}_k\|_2 = \min_{p \in P^k, p(0) = 1} \|p(AC^{(\ell)})\tilde{r}_0\|_2 \leq \left( \min_{p \in P^k, p(0) = 1} \max_{\lambda \in \sigma(AC^{(\ell)})} |p(\lambda)| \right) \|\tilde{r}_0\|_2.$$ 

Since the eigenvalues not equal to zero of $AC^{(\ell)}$ are in the circle with radius $\rho(H)^{\ell} < 1$ with center at 1, [4, Theorems 2, 5] gives the bound $\nu(H)^{k\ell}$ of the first factor. Similarly to the error bound of CG using the condition number of the coefficient matrix, the residual bound of MR is obtained (cf. [36, Section 6.11.3]).

From Theorem 2.11, the convergence of MR preconditioned by inner iterations is expected to be fast as the spectral radius is small and/or the number of inner iterations are large.

We compare the convergence of MR preconditioned by inner iterations with the stationary iterative method alone that is used as inner iterations for MR. If their (inner) iteration matrices are the same and semiconvergent, then the convergence of MR preconditioned by inner iterations is not worse in terms of the number of outer iterations vs. the residual norm. This is because the convergence factor of the stationary iterative method is $\nu(H)^k$, which is larger than the factors in (2.4). However, their computational costs of each iteration are not the same, the total costs required to attain a certain stopping criterion are easily comparable in theory.

Since it is assumed in Theorem 2.11 that $H$ is semiconvergent, which is weaker than that $M + N$ is SD, Theorem 2.11 looses generality concerning the indefiniteness. We showed Theorem 2.11 for the application of MR to the normal equations, whose coefficient matrices are SPSD.

### 2.5 Specific inner-iteration preconditioning methods.

Theorem 2.8 gives insights for justifying the use of specific stationary iterative methods as inner-iteration preconditioning for CG and MR for solving SPSD and indefinite systems, respectively.
Lemma 2.12. Let \( A = A^T \), \( B \) SPD and \( M = \omega^{-1}B \). Denote the largest eigenvalue of \( B^{-\frac{1}{2}}AB^{-\frac{1}{2}} \) by \( \lambda_{\text{max}} \). Then, \( 2M - A \) is SPD if and only if \( \omega \in (0, 2/\lambda_{\text{max}}) \) for \( \lambda_{\text{max}} > 0 \), \( \omega \not\in [2/\lambda_{\text{max}}, 0] \) for \( \lambda_{\text{max}} < 0 \), or \( \omega > 0 \) for \( \lambda_{\text{max}} = 0 \).

Proof. Denote an eigenvalue of \( B^{-\frac{1}{2}}AB^{-\frac{1}{2}} \) by \( \lambda \). Then the corresponding eigenvalue of \( 2\omega^{-1}I - B^{-\frac{1}{2}}AB^{-\frac{1}{2}} \equiv 2\omega^{-1}B - A = 2M - A \) is \( 2\omega^{-1} - \lambda \). From \( 2\omega^{-1} - \lambda > 0 \) for all \( \lambda \in \sigma(B^{-\frac{1}{2}}AB^{-\frac{1}{2}}) \), we have the intervals of \( \omega \) for the positive definiteness of \( 2M - A \). \( \square \)

From Lemma 2.12 with the splitting matrices \( B = I \) and \( D \) SPD, we obtain the interval of the relaxation parameter \( \omega \) for the definiteness of the Richardson and JOR inner-iteration preconditioning matrices \( C^{(l)} \) for \( l \) even. We omit the details to avoid redundancy. From Lemma 2.12, with an SPD splitting matrix not necessarily diagonal, we can generalized JOR.

Next, consider SSOR applied to (1.1). Let \( (\omega^{-1}D + L) \) be the splitting matrix of \( A \) for the forward sweep of SSOR and \( (\omega^{-1}D + L^T) \) be that of \( A \) for the backward sweep.

Theorem 2.13. Assume that \( D \) is SPD. Then, the SSOR splitting matrix \( M = \omega^{-1}(2 - \omega)^{-1}(D + \omega L)D^{-1}(D + \omega L^T) \) of \( A \) is nonsingular if and only if \( \omega \not\in [0, 2] \). For \( l \) odd, the SSOR inner-iteration preconditioning matrix is SPD if and only if \( \omega \in (0, 2) \). Let \( \mu = \lambda_{\text{min}}[D^{-\frac{1}{2}}(L + L^T)D^{-\frac{1}{2}}] + 1 \)

\[
\rho_s = \lambda_{\text{max}}(D^{-\frac{1}{2}}(L + L^T)D^{-\frac{1}{2}}) + 2\lambda_{\text{max}}(D^{-\frac{1}{2}}LD^{-\frac{1}{2}}) + 1.
\]

Then, for \( l \) even, the SSOR inner-iteration preconditioning matrix is SPD if

\[
\begin{align*}
\omega &\in (0, (1 - \sqrt{1 - 2\mu})/\mu) \quad \text{for} \quad \mu < 1/2, \mu \neq 0, \\
\omega &\in (0, 1) \quad \text{for} \quad \mu = 0, \\
\omega &\in (0, 2) \quad \text{for} \quad \mu \geq 1/2, \\
\omega &\not\in [(1 + \sqrt{1 - 2\rho_s})/\rho_s, 2] \quad \text{for} \quad \rho_s < 0, \\
\omega &> 2 \quad \text{for} \quad \rho_s = 0, \\
\omega &\in (2, (1 + \sqrt{1 - 2\rho_s})/\rho_s) \quad \text{for} \quad \rho_s \in (0, 1/2).
\end{align*}
\]

(2.5)

Proof. Since \( \omega^{-1}(2 - \omega)^{-1}(D + \omega L)D^{-1}(D + \omega L^T) \equiv \omega^{-1}(2 - \omega)^{-1}I \), the SSOR splitting matrix of \( A \) is nonsingular if \( \omega \not\in [0, 2] \). For \( l \) odd, from Theorem 2.8, the SSOR inner-iteration preconditioning matrix is SPD if and only if \( \omega \in (0, 2) \). Next, let \( l \) even. Assume \( \omega \neq 0, 2 \). Noting

\[
2M - A = 2\omega^{-1}(2 - \omega)^{-1}(D + \omega L)D^{-1}(D + \omega L^T) - A
\equiv \omega^{-1}(2 - \omega)^{-1}[(\omega^2 - 2\omega + 2)I + \omega^2 D^{-\frac{1}{2}}(L + L^T)D^{-\frac{1}{2}} + 2\omega^2 D^{-\frac{1}{2}}LD^{-\frac{1}{2}}L^TD^{-\frac{1}{2}}],
\]

Let \( \omega \in \mathbb{R} \) hereafter. The splitting matrix \( \omega^{-1}I \) of \( A \) gives the Richardson method for (1.1) if \( \omega \neq 0 \). For odd \( l \), the inner-iteration preconditioning matrix \( C^{(l)} \) of the Richardson method is definite if \( \omega \neq 0 \). Let \( A = L + D + L^T \), where \( L \) is strictly lower triangular and \( D \) is diagonal. Then, the splitting matrix \( \omega^{-1}D \) of \( A \) with \( D \) nonsingular gives JOR for (1.1) if \( \omega \neq 0 \). For odd \( l \), the inner-iteration preconditioning matrix \( C^{(l)} \) of JOR is definite if \( \omega \neq 0 \) and \( D \) is definite. For \( l \) even, we show the following. Note that the splitting \( A = M - N \) gives \( M + N = 2M - A \).
Let
\[ G(\omega) = \omega(2 - \omega)D^{-\frac{1}{2}}(2M - A)D^{-\frac{1}{2}} = (\omega^2 - 2\omega + 2)I + \omega^2D^{-\frac{1}{2}}(L + L^T)D^{-\frac{1}{2}} + 2\omega^2D^{-\frac{1}{2}}LD^{-\frac{1}{2}}L^TD^{-\frac{1}{2}}. \]

If \( v = v(\omega) \) is a real vector such that \( \|v\|_2 = 1 \) and \( G(\omega)v = \lambda v \), then \( \lambda \in \mathbb{R} \) is an eigenvalue of \( G(\omega) \). Note \( \lambda \geq \mu \omega^2 - 2\omega + 2 \) and \( \lambda \leq \mu \omega^2 - 2\omega + 2 \). Noting \( \omega(2 - \omega) > 0 \) for \( \omega \in (0, 2) \), if the first three conditions in (2.5) hold, then the SSOR inner-iteration preconditioning matrix is SPD. Noting \( \omega(2 - \omega) < 0 \) for \( \omega \notin [0, 2] \), if the last three conditions in (2.5) hold, then the SSOR inner-iteration preconditioning matrix is SPD.

Note that the SSOR iteration matrix of \( A \) is SPD with \( D \) SPD and \( \omega \in (0, 2) \) is semiconvergent [11, Theorem 14].

Similar arguments to the above for \( D \) SND and for the case where \( C^{(\ell)} \) is SND hold but we omit the details.

3 Application to least squares problems.

Consider solving linear least squares problems (1.4). We apply results in Section 2 to CGLS, LSQR, and LSMR preconditioned by inner iterations with \( A = A^TA \) and \( b = A^Tb \), and reveal the theory behind the inner-iteration preconditioning [30], [31] in the next subsection.

3.1 Inner-iteration preconditioning.

We give an expression for the preconditioned matrix for CGLS and LSQR with \( \ell \) inner iterations, similarly to Section 2.1. Consider the stationary iterative method applied to \( A^Tz = s_k \) in lines 2 and 6 in [31, Algorithm E.1]. Let \( M \) be nonsingular such that \( A^TA = M - N \). Denote the iteration matrix by \( H = M^{-1}N \). Assume that the initial iterate is \( z^{(0)} = 0 \). Then, the \( \ell \)th iterate of the stationary iterative method is \( z^{(\ell)} = Hz^{(\ell-1)} + M^{-1}s_k = \sum_{i=0}^{\ell-1} H^iM^{-1}s_k, \ell > 0 \). Hence, the preconditioning matrix is \( C^{(\ell)} = \sum_{i=0}^{\ell-1} H^iM^{-1} \). Therefore, the preconditioned matrix is \( C^{(\ell)}A^{(\ell)} = \sum_{i=0}^{\ell-1} H^i(1-H) = 1-H^\ell \).

See [37] for a different formulation of CGLS preconditioned by the SSOR splitting.

Next, consider LSMR preconditioned by inner iterations. The stationary iterative method applied to \( A^Tz = \bar{v}_k \) in lines 3 and 7 in [31, Algorithm E.2] gives the same preconditioning and preconditioned matrices as above. Now we give conditions such that CGLS, LSQR, and LSMR preconditioned by inner iterations determine a least squares solution.

**Theorem 3.1.** Let \( A \in \mathbb{R}^{m \times n} \) and \( M = M^T \) be nonsingular such that \( A^TA = M - N \). Then, CGLS, LSQR, and LSMR preconditioned by \( \ell \) steps of the inner iterations defined above with \( M \) definite for \( \ell \) odd and \( M + N \) definite for \( \ell \) even, respectively, determine a solution of \( \min_{x \in \mathbb{R}^n} \|b - Ax\|_2 \) for all \( b \in \mathbb{R}^m \) and for all \( x_0 \in \mathbb{R}^n \).

**Proof.** Since \( A^TA \) is SPD, the following hold from Theorem 2.8. For \( \ell \) odd, \( C^{(\ell)} \) is SPD (SND) if and only if \( M \) is SPD (SND). For \( \ell \) even, \( C^{(\ell)} \) is SPD (SND) if and only if \( M + N \) is SPD (SND). Hence, Theorems 2.10 and 2.10 complete the proof.

Remark that this theorem holds whether \( A \) is of full-rank or rank-deficient, and whether \( A \) is overdetermined or underdetermined, i.e., unconditionally with respect to \( A \). We have bounds of these methods from Section 2.4.
3.2 Specific inner-iteration preconditioning methods.

There are efficient implementations of inner-iteration preconditioning without explicitly forming $AA^T$ such as the Richardson-NE, Cimmino-NE, and NE-SSOR methods [31, Appendix D], which are mathematically equivalent to the Richardson method, JOR, and SSOR applied to the normal equations of the second kind, respectively. CGLS preconditioned by one step of NE-SSOR was considered in [5].

Let $A^TA = L + D + L^T$, where $L$ is strictly lower triangular and $D$ is diagonal. Assume that $A$ has no zero columns. Then, $D$ is SPD. If $A = A^TA$ and $b = A^Tb$ in Section 2.5, then we obtain the intervals of the parameter values of Richardson-NE, Cimmino-NE, and NE-SSOR such that their inner-iteration preconditioning matrices are SD. Thus, from Theorem 3.1, CGLS, LSQR, and LSMR preconditioned by these inner iterations with relaxation parameters within the intervals determines a solution of $\min_{x \in \mathbb{R}^n} \|b - Ax\|_2$ for all $b \in \mathbb{R}^m$ and for all $x_0 \in \mathbb{R}^n$.

4 Application to minimum-norm solution problems.

Consider solving minimum-norm solution problems (1.5). Results in Section 2 can also be applied to CGNE and MRNE preconditioned by the Richardson-NE, Cimmino-NE, and NE-SSOR inner iterations with $A = A^TA$ and $b = b$. CGNE preconditioned by one step of NE-SSOR was considered in [5]. We generalize this to a multistep version of NE-SSOR.

4.1 Inner-iteration preconditioning.

We give an expression for the inner-iteration preconditioning and preconditioned matrices for CGNE with $\ell$ inner iterations. Consider the stationary iterative method applied to $AA^T z = r_k$ in lines 2 and 6 in [31, Algorithm E.3]. Let $M$ be nonsingular such that $AA^T = M - N$. Denote the iteration matrix by $H = M^{-1}N$. Assume that the initial iterate is $z^{(0)} = 0$. Then, the $\ell$th iterate of the stationary iterative method is $z^{(\ell)} = H z^{(\ell-1)} + M^{-1}r_k = \sum_{i=0}^{\ell-1} H^i M^{-1} r_k$, $\ell > 0$. Hence, the preconditioning and preconditioned matrices are $C^{(\ell)} = \sum_{i=0}^{\ell-1} H^i M^{-1}$ and $C^{(\ell)} AA^T = \sum_{i=0}^{\ell-1} H^i (I - H) = I - H^\ell$, respectively.

Next, consider MRNE preconditioned by inner iterations. The stationary iterative method applied to $AA^T u = c$ in lines 2 and 6 [31, Algorithm E.4] gives the same preconditioning and preconditioned matrices as above. Since $AA^T$ is SPSD, the following hold from Theorem 2.8. For $\ell$ odd, $C^{(\ell)}$ is SPD (SND) if and only if $M$ is SPD (SND). For $\ell$ even, $C^{(\ell)}$ is SPD (SND) if and only if $M + N$ is SPD (SND). Thus, we obtain the following similarly to Theorem 3.1.

**Theorem 4.1.** Let $A \in \mathbb{R}^{m \times n}$ and $M = M^T$ be nonsingular such that $AA^T = M - N$. Then, the CGNE and MRNE methods preconditioned by $\ell$ steps of the inner iterations defined above with $M$ definite for $\ell$ odd and $M + N$ definite for $\ell$ even, respectively, determine a solution of $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathcal{R}(A)$.

Remark that this theorem holds whether $A$ is of full-rank or rank-deficient, and whether $A$ is overdetermined or underdetermined, i.e., unconditionally with respect to $A$. We have bounds of these methods from Section 2.4.
4.2 Specific inner-iteration preconditioning methods.

Let $AA^T = L + D + L^T$, where $L$ is strictly lower triangular and $D$ is diagonal. Assume that $A$ has no zero rows. Then, $D$ is SPD. If $A = AA^T$ and $b = b$ in Section 2.5, then we obtain the intervals of the parameter values of Richardson-NE, Cimmino-NE, and NE-SSOR such that their inner-iteration preconditioning matrices are SD. Thus, from Theorem 4.1, CGNE and MRNE preconditioned by these inner iterations with relaxation parameters within the intervals determines the pseudo-inverse solution of $Ax = b$ for all $b \in \mathcal{R}(A)$ and for all $x_0 \in \mathcal{R}(A^T)$.

5 Conclusions.

We considered applying stationary iterative methods with a symmetric splitting matrix as inner-iteration preconditioning to Krylov subspace methods. We gave a necessary and sufficient condition such that the inner-iteration preconditioning matrix is definite, and show that CG and MR preconditioned by the inner iterations determines a solution of symmetric linear systems including the singular case. Applying these results to CGLS, LSQR, LSMR, CGNE, and MRNE preconditioned by inner iterations, and we guaranteed using these methods for solving least squares and minimum-norm solution problems whose coefficient matrices are not necessarily of full rank.

Acknowledgement

The author would like to thank Professor Ken Hayami and Doctor Miroslav Rozložník for their valuable comments.

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