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A Class of Preconditioners for Large Indefinite Linear Systems, as by-product of Krylov subspace Methods: Part I*

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Abstract. We propose a class of preconditioners, which are also tailored for symmetric linear systems from linear algebra and nonconvex optimization. Our preconditioners are specifically suited for *large* linear systems and may be obtained as *by-product* of Krylov subspace solvers. Each preconditioner in our class is identified by setting the values of a pair of parameters and a scaling matrix, which are user-dependent, and may be chosen according with the structure of the problem in hand. We provide theoretical properties for our preconditioners. In particular, we show that our preconditioners both shift some eigenvalues of the system matrix to controlled values, and they tend to reduce the modulus of most of the other eigenvalues. In a companion paper we study some structural properties of our class of preconditioners, and report the results on a significant numerical experience.

Keywords: Preconditioners, large indefinite linear systems, large scale nonconvex optimization, Krylov subspace methods.

JEL Classification Numbers: C44, C61.

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1 Introduction

We study a class of preconditioners for the solution of large indefinite linear systems, without assuming any sparsity pattern for the system matrix. In many contexts of numerical analysis and nonlinear optimization the iterative efficient solution of sequences of linear systems is sought. Truncated Newton methods in unconstrained optimization, KKT systems, interior point methods, and PDE constrained optimization are just some examples (see e.g. [5]).

In this work we consider the solution of symmetric indefinite linear systems by using preconditioning techniques; in particular, the class of preconditioners we propose uses information collected by Krylov subspace methods, in order to capture the structural properties of the system matrix. We iteratively construct our preconditioners either by using (but not performing) a factorization of the system matrix (see, e.g. [8, 12, 19]), obtained as by product of Krylov subspace methods, or performing a Jordan Canonical form on a *very small size* matrix. We address our preconditioners using a general Krylov subspace method; then, we prove theoretical properties for such preconditioners, and we describe results which indicate how to possibly select the parameters involved in the definition of the preconditioners. The basic idea of our approach is that we apply a Krylov-based method to generate a positive definite *approximation* of the inverse of the system matrix. The latter is then used to build our preconditioners, needing to store just a few vectors, without requiring any product of matrices. Since we collect information from Krylov-based methods, we assume that the entries of the system matrix are not known and the necessary information is gained by using a routine, which computes the product of the system matrix times a vector.

In the companion paper [10] we experience our preconditioners, both within linear algebra and nonconvex optimization frameworks. In particular, we test our proposal on significant linear systems from the literature. Then, we focus on the so called *Newton–Krylov methods*, also known as Truncated Newton methods (see [16] for a survey). In these contexts, both positive definite and indefinite linear systems have been considered.

We recall that in case the optimization problem in hand is nonconvex, i.e. the Hessian matrix of the objective function is possibly indefinite and at least one eigenvalue is negative, the solution of Newton's equations within Truncated Newton schemes may claim for some cares. Indeed, the Krylov-based method used to solve Newton's equation, should be suitably applied considering that, unlike in linear algebra, optimization frameworks require the definition of *descent directions*, which have to satisfy additional properties [6, 17]. In this regard our proposal provides a tool, in order to preserve the latter properties.

The paper is organized as follows: in the next section we describe our class of preconditioners for indefinite linear systems, by using a general Krylov subspace method. Finally, a section of conclusions and future work completes the paper.

As regards the notations, for a $n \times n$ real matrix M we denote with $\Lambda[M]$ the spectrum of M; I_k is the identity matrix of order k. Finally, with $C \succ 0$ we indicate that the matrix C is positive definite, $tr[C]$ and $det[C]$ are the *trace* and the *determinant* of C, respectively, while $\|\cdot\|$ denotes the Euclidean norm.

2 Our class of preconditioners

In this section we first introduce some preliminaries, then we propose our class of preconditioners. Consider the *indefinite* linear system

$$Ax = b, \tag{2.1}$$

where $A \in \mathbb{R}^{n\times n}$ is *symmetric*, n is *large* and $b \in \mathbb{R}^n$. Some real contexts where the latter system requires efficient solvers are detailed in Section 1. Suppose any Krylov subspace method is used for the solution of (2.1), e.g. the Lanczos process or the CG method [12] (but MINRES [18] or Planar-CG methods [13, 7] may be also an alternative choice). They are equivalent as long as $A \succ 0$, whereas the CG, though cheaper, in principle may not cope with the indefinite case. In the next Assumption 2.1 we consider that a finite number of steps, say $h \ll n$, of the Krylov subspace method adopted have been performed.

Assumption 2.1 *Let us consider any Krylov subspace method to solve the symmetric linear system (2.1). Suppose at step h of the Krylov method, with $h \le n-1$, the matrices $R_h \in \mathbb{R}^{n\times h}$, $T_h \in \mathbb{R}^{h\times h}$ and the vector $u_{h+1} \in \mathbb{R}^n$ are generated, such that*

$$AR_h = R_h T_h + \rho_{h+1} u_{h+1} e_h^T, \qquad \rho_{h+1} \in \mathbb{R}, \tag{2.2}$$

$$T_h = \begin{cases} V_h B_h V_h^T, & \text{if } T_h \text{ is indefinite} \\ \\ L_h D_h L_h^T, & \text{if } T_h \text{ is positive definite} \end{cases} \tag{2.3}$$

where

$R_h = (u_1 \cdots u_h)$, $u_i^T u_j = 0$, $\|u_i\| = 1$, $1 \le i \ne j \le h$,

$u_{h+1}^T u_i = 0$, $\|u_{h+1}\| = 1$, $1 \le i \le h$,

T_h is irreducible and nonsingular, with eigenvalues $\mu_1, \ldots, \mu_h$ not all coincident,

$B_h = diag_{1\le i\le h}\{\mu_i\}$, $V_h = (v_1 \cdots v_h) \in \mathbb{R}^{h\times h}$ orthogonal, (μ_i, v_i) is eigenpair of T_h,

$D_h \succ 0$ is diagonal, L_h is unit lower bidiagonal.

Remark 2.1 Note that most of the common Krylov subspace methods for the solution of symmetric linear systems (e.g. the CG, the Lanczos process, etc.) at iteration h may easily satisfy Assumption 2.1. In particular, also observe that from (2.2) we have $T_h = R_h^T A R_h$, so that whenever $A \succ 0$ then $T_h \succ 0$. Since the Jordan Canonical form of T_h in (2.3) is required only when T_h is indefinite, it is important to check when $T_h \succ 0$, without computing the eigenpairs of T_h if unnecessary. On this purpose, note that the Krylov subspace method adopted always provides relation $T_h = L_h D_h L_h^T$, with L_h nonsingular and D_h block diagonal (blocks can be 1×1 or 2×2 at most), even when T_h is indefinite [18, 19, 8]. Thus, checking the eigenvalues of D_h will suggest if the Jordan Canonical form $T_h = V_h B_h V_h^T$ is really needed for T_h, i.e. if T_h is indefinite.

Observe also that from Assumption 2.1 the parameter ρ_{h+1} ma be possibly nonzero, i.e. the subspace $span\{u_1,\dots,u_h\}$ is possibly not an invariant subspace under the transformation by matrix A (thus, in this paper we consider a more general case with respect to [3]).

Remark 2.2 The Krylov subspace method adopted may, in general, perform $m \geq h$ iterations, generating the orthonormal vectors $u_1,\dots,u_m$. Then, we can set $R_h = (u_{\ell_1},\dots,u_{\ell_h})$, where $\{\ell_1,\dots,\ell_h\} \subseteq \{1,\dots,m\}$, and change relations (2.2)-(2.3) accordingly; i.e. Assumption 2.1 may hold selecting any h out of the m vectors (among $u_1,\dots,u_m$) computed by the Krylov subspace method.

Remark 2.3 For relatively small values of the parameter h in Assumption 2.1 (say $h \leq 20$, as often suffices in most of the applications), the computation of the eigenpairs (μ_i, v_i), $i = 1,\dots,h$, of T_h when T_h is indefinite may be extremely fast, with standard codes. E.g. if the CG is the Krylov subspace method used in Assumption 2.1 to solve (2.1), then the `Matlab` [1] (general) function `eigs()` requires as low as $\approx 10^{-4}$ seconds to fully compute all the eigenpairs of T_h, for $h = 20$, on a commercial laptop. In the latter case indeed, the matrix T_h is tridiagonal. Nonetheless, in the separate paper [9] we consider a special case where the request (2.3) on T_h may be considerably weakened under mild assumptions. Moreover, in the companion paper [10] we also prove that for a special choice of the parameter 'a' used in our class of preconditioners (see below), strong theoretical properties may be stated.

On the basis of the latter assumption, we can now define our preconditioners and show their properties. To this aim, considering for the matrix T_h the expression (2.3), we define (see also [11])

$$|T_h| \stackrel{\text{def}}{=} \begin{cases} V_h|B_h|V_h^T, \quad |B_h| = \ diag_{1\leq i\leq h}\{|\mu_i|\}, & \text{if } T_h \text{ is indefinite,} \\ \\ T_h, & \text{if } T_h \text{ is positive definite.} \end{cases}$$

As a consequence, when T_h is indefinite we have $T_h|T_h|^{-1} = |T_h|^{-1}T_h = V_h\hat{I}_hV_h^T$, where the h nonzero diagonal entries of the matrix $\hat{I}_h$ are in the set $\{-1,+1\}$. Furthermore, it is easily seen that $|T_h|$ is positive definite, for any h, and the matrix $|T_h|^{-1}T_h^2|T_h|^{-1} = I_h$ is the identity matrix.

Now let us introduce the following $n \times n$ matrix, which *depends on the real parameter* 'a':

$$\begin{aligned} M_h &\stackrel{\text{def}}{=} (I - R_hR_h^T) + R_h|T_h|R_h^T + a\left(u_{h+1}u_h^T + u_hu_{h+1}^T\right), \qquad\qquad h \leq n-1, \\ &= [R_h \mid u_{h+1} \mid R_{n,h+1}] \left[\begin{array}{c|c} \left(\begin{array}{c|c} |T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right) & 0 \\ \hline 0 & I_{n-(h+1)} \end{array}\right] \left[\begin{array}{c} R_h^T \\ \hline u_{h+1}^T \\ \hline R_{n,h+1}^T \end{array}\right] \end{aligned} \tag{2.4}$$

$$M_n \stackrel{\text{def}}{=} (I - R_nR_n^T) + R_n|T_n|R_n^T = R_n|T_n|R_n^T, \tag{2.5}$$

where R_h and T_h satisfy relations (2.2)-(2.3), $a \in \mathbb{R}$, the matrix $R_{n,h+1} \in \mathbb{R}^{n\times[n-(h+1)]}$ is such that $R_{n,h+1}^TR_{n,h+1} = I_{n-(h+1)}$ and $[R_h \mid u_{h+1} \mid R_{n,h+1}]$ is orthogonal. By (2.4), when

$h \le n-1$, the matrix M_h is the sum of three terms.
It is easily seen that $I - R_h R_h^T$ represents a projector onto the subspace $\mathcal{S}$ orthogonal to the range of matrix R_h, so that $M_h v = v + a(u_{h+1}^T v)u_h$, for any $v \in \mathcal{S}$. Thus, for any $v \in \mathcal{S}$, when either $u_{h+1}^T v = 0$ or $a = 0$, then $M_h v = v$ (or equivalently if M_h is nonsingular $M_h^{-1} v = v$), i.e. the vector v is unaltered by applying M_h (or M_h^{-1}). As a result, if either $a = 0$ or $u_{h+1}^T v = 0$ then M_h behaves as the identity matrix for any vector $v \in \mathcal{S}$.
Using the parameter dependent matrix M_h in (2.4)-(2.5) we are now ready to introduce the following class of preconditioners

$$\begin{aligned} M_h^\sharp(a,\delta,D) &= D\left[I_n - (R_h \mid u_{h+1})(R_h \mid u_{h+1})^T\right] D^T \qquad h \le n-1, \\ &+ (R_h \mid Du_{h+1}) \left(\begin{array}{c|c} \delta^2 |T_h| & a e_h \\ \hline a e_h^T & 1 \end{array}\right)^{-1} (R_h \mid Du_{h+1})^T \qquad (2.6) \\ M_n^\sharp(a,\delta,D) &= R_n |T_n|^{-1} R_n^T. \qquad (2.7) \end{aligned}$$

Theorem 2.1 *Consider any Krylov method to solve the symmetric linear system (2.1). Suppose that Assumption 2.1 holds and the Krylov method performs $h \le n$ iterations. Let $a \in \mathbb{R}$, $\delta \neq 0$, and let the matrix $D \in \mathbb{R}^{n\times n}$ be such that $[R_h \mid Du_{h+1} \mid DR_{n,h+1}]$ is nonsingular, where $R_{n,h+1}R_{n,h+1}^T = I_n - (R_h \mid u_{h+1})(R_h \mid u_{h+1})^T$. Then, we have the following properties:*

a) the matrix $M_h^\sharp(a,\delta,D)$ is symmetric. Furthermore

- *when $h \le n-1$, for any $a \in \mathbb{R} - \{\pm\delta(e_h^T |T_h|^{-1} e_h)^{-1/2}\}$, $M_h^\sharp(a,\delta,D)$ is nonsingular;*
- *when $h = n$ the matrix $M_h^\sharp(a,\delta,D)$ is nonsingular;*

b) the matrix $M_h^\sharp(a,\delta,D)$ coincides with M_h^{-1} as long as either $D = I_n$ and $\delta = 1$, or $h = n$;

c) for $|a| < |\delta|(e_h^T |T_h|^{-1} e_h)^{-1/2}$ the matrix $M_h^\sharp(a,\delta,D)$ is positive definite. Moreover, if $D = I_n$ the spectrum $\Lambda[M_h^\sharp(a,\delta,I_n)]$ is given by

$$\Lambda[M_h^\sharp(a,\delta,I_n)] = \Lambda\left[\left(\begin{array}{c|c} \delta^2 |T_h| & a e_h \\ \hline a e_h^T & 1 \end{array}\right)^{-1}\right] \cup \Lambda\left[I_{n-(h+1)}\right];$$

d) when $h \le n-1$:

- *if D is nonsingular then $M_h^\sharp(a,\delta,D)A$ has at least $(h-3)$ singular values equal to $+1/\delta^2$;*
- *if D is nonsingular and $a = 0$ then the matrix $M_h^\sharp(a,\delta,D)A$ has at least $(h-2)$ singular values equal to $+1/\delta^2$;*

e) when $h = n$, then $M_n^\sharp(a,\delta,D) = M_n^{-1}$, $\Lambda[M_n] = \Lambda[|T_n|]$ and $\Lambda[M_n^{-1}A] = \Lambda[AM_n^{-1}] \subseteq \{-1,+1\}$, i.e. the n eigenvalues of the preconditioned matrix $M_h^\sharp(a,\delta,D)A$ are either $+1$ or -1.

Proof: Let $N = [R_h \mid Du_{h+1} \mid DR_{n,h+1}]$, where N is nonsingular by hypothesis. Observe that for $h \le n-1$ the preconditioners $M_h^\sharp(a,\delta,D)$ may be rewritten as

$$M_h^\sharp(a,\delta,D) = N \left[\begin{array}{c|c} \left(\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right)^{-1} & 0 \\ \hline 0 & I_{n-(h+1)} \end{array} \right] N^T, \qquad h \le n-1. \tag{2.8}$$

The property a) follows from the symmetry of T_h. In addition, observe that $R_{n,h+1}^T R_{n,h+1} = I_{n-(h+1)}$. Thus, from (2.8) the matrix $M_h^\sharp(a,\delta,D)$ is nonsingular if and only if the matrix

$$\left(\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right) \tag{2.9}$$

is invertible. Furthermore, by a direct computation we observe that for $h \le n-1$ the following identity holds

$$\left(\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right) = \left(\begin{array}{c|c} I_h & 0 \\ \hline \frac{a}{\delta^2}e_h^T|T_h|^{-1} & 1 \end{array}\right) \left(\begin{array}{c|c} \delta^2|T_h| & 0 \\ \hline 0 & 1-\frac{a^2}{\delta^2}e_h^T|T_h|^{-1}e_h \end{array}\right) \left(\begin{array}{c|c} I_h & \frac{a}{\delta^2}|T_h|^{-1}e_h \\ \hline 0 & 1 \end{array}\right). \tag{2.10}$$

Thus, since T_h is nonsingular and $\delta \ne 0$, for $h \le n-1$ the determinant of matrix (2.9) is nonzero if and only if $a \ne \pm\delta(e_h^T|T_h|^{-1}e_h)^{-1/2}$. Finally, for $h = n$ the matrix $M_h^\sharp(a,\delta,D)$ is nonsingular, since R_n and T_n are nonsingular in (2.7).

As regards b), recalling that $R_h^T R_h = I_h$ and $|T_h|$ is nonsingular from Assumption 2.1, when $h \le n-1$ relations (2.4) and (2.8) trivially yield the result, as well as (2.5) and (2.7) for the case $h = n$.

As regards c), observe that from (2.8) the matrix $M_h^\sharp(a,\delta,D)$ is positive definite, as long as the matrix (2.9) is positive definite. Thus, from (2.10) and relation $|T_h| \succ 0$ we immediately infer that $M_h^\sharp(a,\delta,D)$ is positive definite as long as $|a| < |\delta|(e_h^T|T_h|^{-1}e_h)^{-1/2}$. Moreover, we recall that when $D = I_n$ then N is orthogonal.

Item d) may be proved by first computing the eigenvalues of the matrix

$$\left[M_h^\sharp(a,\delta,D)A\right]\left[M_h^\sharp(a,\delta,D)A\right]^T = M_h^\sharp(a,\delta,D)A^2M_h^\sharp(a,\delta,D).$$

On this purpose, for $h \le n-1$ we have for $M_h^\sharp(a,\delta,D)A^2M_h^\sharp(a,\delta,D)$ the expression (see (2.8))

$$\begin{aligned} M_h^\sharp(a,\delta,D)A^2M_h^\sharp(a,\delta,D) &= \\ N \left[\begin{array}{c|c} \left(\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right)^{-1} & 0 \\ \hline 0 & I_{n-(h+1)} \end{array} \right] C \left[\begin{array}{c|c} \left(\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right)^{-1} & 0 \\ \hline 0 & I_{n-(h+1)} \end{array} \right] N^T \end{aligned} \tag{2.11}$$

where $C \in \mathbb{R}^{n\times n}$, with

$$C = N^TA^2N = \left[\begin{array}{c|c|c} R_h^TA^2R_h & R_h^TA^2Du_{h+1} & R_h^TA^2DR_{n,h+1} \\ \hline u_{h+1}^TD^TA^2R_h & u_{h+1}^TD^TA^2Du_{h+1} & u_{h+1}^TD^TA^2DR_{n,h+1} \\ \hline R_{n,h+1}^TD^TA^2R_h & R_{n,h+1}^TD^TA^2Du_{h+1} & R_{n,h+1}^TD^TA^2DR_{n,h+1} \end{array}\right].$$

From (2.2) and the symmetry of T_h we obtain

$$\begin{aligned} R_h^TA^2R_h &= (AR_h)^T(AR_h) \;=\; (R_hT_h + \rho_{h+1}u_{h+1}e_h^T)^T(R_hT_h + \rho_{h+1}u_{h+1}e_h^T) \\ &= T_h^2 + \rho_{h+1}^2 e_h e_h^T \\ R_h^TA^2Du_{h+1} &= (AR_h)^TADu_{h+1} \;=\; (R_hT_h + \rho_{h+1}u_{h+1}e_h^T)^TADu_{h+1} \\ &= T_hR_h^TADu_{h+1} + \rho_{h+1}(u_{h+1}^TADu_{h+1})e_h \\ &= T_h(R_hT_h + \rho_{h+1}u_{h+1}e_h^T)^TDu_{h+1} + \rho_{h+1}(u_{h+1}^TADu_{h+1})e_h \\ &= v_1 \qquad (2.12) \\ R_h^TA^2DR_{n,h+1} &= V_1 \\ u_{h+1}^TD^TA^2Du_{h+1} &= c \\ u_{h+1}^TD^TA^2DR_{n,h+1} &= v_2^T \\ R_{n,h+1}^TD^TA^2DR_{n,h+1} &= V_2, \end{aligned} \qquad (2.13)$$

so that

$$C \;=\; \left[\begin{array}{c|c|c} T_h^2 + \rho_{h+1}^2e_he_h^T & v_1 & V_1 \\ \hline v_1^T & c & v_2^T \\ \hline V_1^T & v_2 & V_2 \end{array}\right].$$

Moreover, from (2.10) we can readily infer that

$$\begin{aligned} &\left[\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right]^{-1} \;= \\ &\left(\begin{array}{c|c} I_h & -\frac{a}{\delta^2}|T_h|^{-1}e_h \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} \frac{1}{\delta^2}|T_h|^{-1} & 0 \\ \hline 0 & \frac{1}{1-\frac{a^2}{\delta^2}e_h^T|T_h|^{-1}e_h} \end{array}\right)\left(\begin{array}{c|c} I_h & 0 \\ \hline -\frac{a}{\delta^2}e_h^T|T_h|^{-1} & 1 \end{array}\right) \;= \\ &\left(\begin{array}{c|c} \frac{1}{\delta^2}|T_h|^{-1} - \frac{a}{\delta^4}\omega|T_h|^{-1}e_he_h^T|T_h|^{-1} & \frac{\omega}{\delta^2}|T_h|^{-1}e_h \\ \hline \frac{\omega}{\delta^2}e_h^T|T_h|^{-1} & -\frac{\omega}{a} \end{array}\right), \end{aligned} \qquad (2.14)$$

with

$$\omega = -\frac{a}{1 - \frac{a^2}{\delta^2}e_h^T|T_h|^{-1}e_h}. \qquad (2.15)$$

Now, recalling that $N = [R_h \mid Du_{h+1} \mid DR_{n,h+1}]$, for any $h \leq n-1$ we obtain from (2.11)

$$\begin{aligned} &M_h^\sharp(a,\delta,D)A^2M_h^\sharp(a,\delta,D) \;= \\ &\qquad N\left[\begin{array}{c|c} \left[\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right]^{-1}\left[\begin{array}{c|c} T_h^2 + \rho_{h+1}^2e_he_h^T & v_1 \\ \hline v_1^T & c \end{array}\right]\left[\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right]^{-1} & \vdots \\ \hline \cdots & \cdot \end{array}\right]N^T, \end{aligned}$$

where the *dots* indicate matrices whose computation is not relevant to our purposes.

Now, considering the last relation, we focus on computing the submatrix $H_{h\times h}$ corresponding to the first h rows and h columns of the matrix

$$\left[\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right]^{-1} \left[\begin{array}{c|c} T_h^2+\rho_{h+1}^2 e_h e_h^T & v_1 \\ \hline v_1^T & c \end{array}\right] \left[\begin{array}{c|c} \delta^2|T_h| & ae_h \\ \hline ae_h^T & 1 \end{array}\right]^{-1}. \tag{2.16}$$

After a brief computation, from (2.14) and (2.16) we obtain for the submatrix $H_{h\times h}$

$$\begin{aligned} H_{h\times h} \;=\; & \left[\left(\frac{1}{\delta^2}|T_h|^{-1} - \frac{a}{\delta^4}\omega|T_h|^{-1}e_h e_h^T|T_h|^{-1}\right)\left(T_h^2+\rho_{h+1}^2 e_h e_h^T\right) + \right. \\ & \left. \frac{\omega}{\delta^2}|T_h|^{-1}e_h v_1^T\right]\cdot\left[\frac{1}{\delta^2}|T_h|^{-1} - \frac{a}{\delta^4}\omega|T_h|^{-1}e_h e_h^T|T_h|^{-1}\right] + \\ & \left[\left(\frac{1}{\delta^2}|T_h|^{-1} - \frac{a}{\delta^4}\omega|T_h|^{-1}e_h e_h^T|T_h|^{-1}\right)v_1 + \frac{\omega}{\delta^2}c|T_h|^{-1}e_h\right]\cdot\frac{\omega}{\delta^2}e_h^T|T_h|^{-1}, \end{aligned}$$

and for the case of T_h indefinite, from (2.3) we obtain (a similar analysis holds for the case $T_h \succ 0$, too)

$$\begin{aligned} H_{h\times h} \;=\; & \left[\frac{1}{\delta^2}V_h\hat{I}_hV_h^TT_h + \frac{\rho_{h+1}^2}{\delta^2}|T_h|^{-1}e_he_h^T - \frac{a}{\delta^4}\omega|T_h|^{-1}e_he_h^TV_h\hat{I}_hV_h^TT_h\right. \\ & \left. - \frac{a}{\delta^4}\omega\rho_{h+1}^2e_h^T|T_h|^{-1}e_h|T_h|^{-1}e_he_h^T + \frac{\omega}{\delta^2}|T_h|^{-1}e_hv_1^T\right]\cdot\left[\frac{1}{\delta^2}|T_h|^{-1} - \frac{a}{\delta^4}\omega|T_h|^{-1}e_he_h^T|T_h|^{-1}\right] \\ & + \frac{\omega}{\delta^2}\left[\frac{1}{\delta^2}|T_h|^{-1}v_1 - \frac{a}{\delta^4}\omega|T_h|^{-1}e_he_h^T|T_h|^{-1}v_1 + \frac{\omega}{\delta^2}c|T_h|^{-1}e_h\right]e_h^T|T_h|^{-1}. \end{aligned}$$

Recalling that $(V_h\hat{I}_hV_h^T)(V_h\hat{I}_hV_h^T) = I_h$ (so that $e_h^T(V_h\hat{I}_hV_h^T)(V_h\hat{I}_hV_h^T)e_h = 1$), from the last relation we finally have for $H_{h\times h}$ the expression

$$\begin{aligned} H_{h\times h} \;=\; & \frac{1}{\delta^4}\left\{I_h + \left[\beta|T_h|^{-1}e_h - \frac{a\omega}{\delta^2}e_h + \omega|T_h|^{-1}v_1\right]e_h^T|T_h|^{-1}\right. \\ & \left. +\; \omega|T_h|^{-1}e_h\left[v_1^T|T_h|^{-1} - \frac{a}{\delta^2}e_h^T\right]\right\}, \end{aligned} \tag{2.17}$$

where

$$\begin{aligned} \beta \;=\; & \rho_{h+1}^2 - 2\frac{a}{\delta^2}\omega\rho_{h+1}^2(e_h^T|T_h|^{-1}e_h) + \frac{a^2\omega^2}{\delta^4} \\ & + \frac{a^2}{\delta^4}\omega^2\rho_{h+1}^2(e_h^T|T_h|^{-1}e_h)^2 - \; 2\frac{a}{\delta^2}\omega^2(e_h^T|T_h|^{-1}v_1) + \omega^2 c. \end{aligned} \tag{2.18}$$

Let us now define the subspace (see the vectors which define the dyads in relation (2.17))

$$\mathcal{T}_2 = span\left\{|T_h|^{-1}e_h\;,\;\omega\left[|T_h|^{-1}v_1 - \frac{a}{\delta^2}e_h\right]\right\}. \tag{2.19}$$

Observe that when $D = I_n$ then from (2.12) $v_1 = \rho_{h+1}\left[T_h + (u_{h+1}^TAu_{h+1})I_h\right]e_h$. Thus, from (2.19) the subspace $\mathcal{T}_2$ has dimension 2, unless *(i)* $D = I_n$ and T_h is proportional to I_h,

(ii) $a = 0$ (which also implies from (2.15) $\omega = 0$).

We analyze separately the two cases. The condition *(i)* cannot hold since (2.2) would imply that the vector Au_i is proportional to u_i, $i = 1, \dots, h-1$, i.e. the Krylov subspace method had to stop at the very first iteration, since the Krylov subspace generated at the first iteration did not change. As a consequence, considering any subspace $\mathcal{S}_{h-2} \subseteq \mathbb{R}^n$, such that $\mathcal{S}_{h-2} \bigoplus \mathcal{T}_2 = \mathbb{R}^n$, we can select any orthonormal basis $\{s_1, \dots, s_{h-2}\}$ of the subspace $\mathcal{S}_{h-2}$ so that (see (2.17)) the $h-2$ vectors $\{s_1, \dots, s_{h-2}\}$ can be thought as (the first) $h-2$ eigenvectors of the matrix $H_{h\times h}$, corresponding to the eigenvalue $+1/\delta^4$.
Now, recalling that the submatrix $H_{h\times h}$ corresponds to the first h rows and h columns of the matrix $M_h^\sharp(a,\delta,D)A^2 M_h^\sharp(a,\delta,D)$, from the *Cauchy interlacing property* for the eigenvalues of a real symmetric matrix [4], the matrix $M_h^\sharp(a,\delta,D)A^2 M_h^\sharp(a,\delta,D)$ has at least $h-3$ eigenvalues equal to $+1/\delta^4$. Thus, the matrix $M_h^\sharp(a,\delta,D)A$ has at least $h-3$ singular values equal to $+1/\delta^2$, which proves the first statement of d).
As regards the case (ii) with $a = 0$, observe that by the definition (2.15) of ω, $a = 0$ implies $\omega = 0$, and from relations (2.17)-(2.18), for any D we have $H_{h\times h} = 1/\delta^4[I_h + \rho_{h+1}^2 |T_n|^{-1} e_h e_h^T |T_n|^{-1}]$. Thus, the subspace $\mathcal{T}_2$ in (2.19) reduces to $\mathcal{T}_1 = span\{|T_h|^{-1}e_h\}$. Now, reasoning as in the case (i) (where $D = I_n$, with T_h proportional to I_h), we conclude that the matrix $M_h^\sharp(a,\delta,D)A$ has at least $(h-2)$ singular values equal to $+1/\delta^2$.

As regards item e), observe that for $h = n$ the matrix R_n is orthogonal, so that by (2.5) and (2.7) $\Lambda[M_h^\sharp(a,\delta,D)] = \Lambda[M_h^{-1}] = \Lambda[|T_h|^{-1}]$. Furthermore, by (2.2) and (2.7) we have for the case of T_h indefinite (a similar analysis holds for the case $T_h \succ 0$, too)

$$M_n^\sharp(a,\delta,D)A = M_n^{-1}A = R_n|T_n|^{-1}R_n^T R_n T_n R_n^T = R_n V_n \hat{I}_n V_n^T R_n^T = (R_n V_n)\hat{I}_n(R_n V_n)^T. \tag{2.20}$$

Since both R_n and V_n are orthogonal so is the matrix R_nV_n; thus, relation (2.20) proves that $M_n^\sharp(a,\delta,D)A$ has all the n eigenvalues in the set $\{-1,+1\}$. □

Remark 2.4 Note that of course the matrix $R_{n,h+1}$ in the statement of Theorem 2.1 always exists, such that $[R_h \mid u_{h+1} \mid R_{n,h+1}]$ is orthogonal. However, $R_{n,h+1}$ is neither built nor used in (2.6)-(2.7), and it is introduced only for theoretical purposes. Furthermore, it is easy to see that since $[R_h \mid u_{h+1} \mid R_{n,h+1}]$ is orthogonal, any nonsingular diagonal matrix D may be used in order to satisfy the hypotheses of Theorem 2.1.

Remark 2.5 Observe that the introduction of the nonsingular matrix D in (2.6) addresses a very general structure for the preconditioner $M_h^\sharp(a,\delta,D)$. As an example, setting $h = 0$ we have $M_h^\sharp(a,\delta,D) = DD^T \succ 0$, so that the preconditioner $M_h^\sharp(a,\delta,D)$ will encompass several classes of preconditioners from the literature (e.g. diagonal banded and block diagonal preconditioners [18]), even though no information is provided by the Krylov subspace method. On the other hand, with the choice $D = I_n$ and $\delta = 1$ the preconditioner $M_h^\sharp(a,1,I_n)$ can be regarded as an approximate inverse preconditioner [18], without any scaling. Finally, though the choice $\delta = 1$ in (2.6) seems the most obvious, numerical reasons related to formula (2.14) and to the condition number of $M_h^\sharp(a,\delta,D)A$ may suggest other values for the parameter 'δ'. In the companion paper [10] we give motivations for the latter conclusion.

It is possible to show that trying to introduce a slightly more general structure of $M_h^\sharp(a,\delta,D)$, where the parameter 'δ' is replaced by a scaling (diagonal) matrix $\Delta \in \mathbb{R}^{h\times h}$ (used to *balance* the matrix $|T_h|$), the item *d)* of Theorem 2.1 may not be fulfilled. The next result summarizes the properties of our class of preconditioners, for a very simple and opportunistic choice of the parameters 'a', 'δ' and matrix 'D'.

Corollary 2.2 *Consider any Krylov method to solve the symmetric linear system (2.1). Suppose that Assumption 2.1 holds and the Krylov method performs $h \le n$ iterations. Then, setting $a = 0$, $\delta = 1$ and $D = I_n$ in Theorem 2.1 the preconditioner*

$$\begin{aligned} M_h^\sharp(0,1,I_n) &= \left[I_n - (R_h \mid u_{h+1})(R_h \mid u_{h+1})^T \right] \\ &\quad + (R_h \mid u_{h+1}) \left(\begin{array}{c|c} |T_h| & 0 \\ \hline 0 & 1 \end{array} \right)^{-1} (R_h \mid u_{h+1})^T \end{aligned} \tag{2.21}$$

$$M_n^\sharp(0,1,I_n) = R_n |T_n|^{-1} R_n^T, \tag{2.22}$$

is such that

a) *the matrix $M_h^\sharp(0,1,I_n)$ is symmetric and nonsingular for any $h \le n$;*

b) *the matrix $M_h^\sharp(0,1,I_n)$ coincides with M_h^{-1}, for any $h \le n$;*

c) *the matrix $M_h^\sharp(0,1,I_n)$ is positive definite. Moreover, its spectrum $\Lambda[M_h^\sharp(0,1,I_n)]$ is given by*

$$\Lambda[M_h^\sharp(0,1,I_n)] = \Lambda\left[|T_h|^{-1}\right] \cup \Lambda\left[I_{n-h}\right];$$

d) *when $h \le n-1$, then the matrix $M_h^\sharp(0,1,I_n)A$ has at least $(h-2)$ singular values equal to $+1$;*

e) *when $h = n$, then $\Lambda[M_n] = \Lambda[|T_n|]$ and $\Lambda[M_n^\sharp(0,1,I_n)A] = \Lambda[M_n^{-1}A] = \Lambda[AM_n^{-1}] \subseteq \{-1,+1\}$, i.e. the n eigenvalues of $M_h^\sharp(0,1,I_n)A$ are either $+1$ or -1.*

Proof: The result is directly obtained from (2.4)-(2.5) and Theorem 2.1, with $a = 0$, $\delta = 1$ and $D = I_n$. □

Remark 2.6 Observe that the case $h \approx n$ in Theorem 2.1 and Corollary 2.2 is of scarce interest for large scale problems. Indeed, in the literature of preconditioners the values of 'h' typically do not exceed $10 \div 20$ [14, 15]. Moreover, for small values of h the computation of the inverse matrix

$$\left(\begin{array}{c|c} \delta^2 |T_h| & a e_h \\ \hline a e_h^T & 1 \end{array} \right)^{-1}, \tag{2.23}$$

in order to provide $M_h^\sharp(a,\delta,I_n)$ or $M_h^\sharp(a,\delta,D)$, may be cheaply performed when T_h is either indefinite or positive definite. In the former case Remark 2.3 and relation (2.14) will provide the result. In the latter case it suffices to use (2.14). Thus, the overall cost (number of flops) for computing (2.23) is mostly due to the computational burden of $|T_h|^{-1}$. However, with a better insight and considering that our preconditioners are suited for large scale problems, observe that the application of our proposal only requires to compute the inverse matrix (2.23) times a real $(h+1)$-dimensional vector. Indeed, Krylov subspace methods never use directly matrices during their recursion. Thus, the computational core of computing the matrix (2.23) times a vector is the product $|T_h|^{-1}u$, where $u \in \mathbb{R}^h$. In this regard, we have the following characterization:

- if T_h is **indefinite** then $|T_h|^{-1}u = (V_h|B_h|V_h^T)^{-1}u = V_h^T|B_h|^{-1}V_h u$, and recalling that B_h is at most 2×2 block diagonal, the cost $\mathcal{C}(|T_h|^{-1}u)$ of calculating the product $|T_h|^{-1}u$ (not including the cost to compute the Jordan Canonical form of T_h), is given by $\mathcal{C}(|T_h|^{-1}u) = O(h^2)$;

- if T_h is **positive definite** then $|T_h|^{-1}u = (L_h D_h L_h^T)^{-1}u = L_h^{-T} D_h^{-1} L_h^{-T} u$. Considering the results in Section 4 of [9], we have that again the cost $\mathcal{C}(|T_h|^{-1}u)$ of computing the product $|T_h|^{-1}u$, is given by $\mathcal{C}(|T_h|^{-1}u) = O(h^2)$.

Remark 2.7 The choice of the parameters 'δ' and 'a', and the matrix 'D' is problem dependent. In particular, 'δ' and 'a' may be set in order to impose conditions like the following (which tend to force the clustering of the eigenvalues of matrix $H_{(h+1)\times(h+1)}$ or $H_{h\times h}$ -see (2.16)- near $+1$ or near -1):

$$\begin{array}{ll} \det\left[H_{(h+1)\times(h+1)}\right] = 1, & tr\left[H_{(h+1)\times(h+1)}\right] = h+1, \\ \det\left[H_{h\times h}\right] = 1, & tr\left[H_{h\times h}\right] = h. \end{array}$$

Nonetheless, also the choice $a = 0$ seems appealing, as described in the companion paper [10]. Finally, observe that depending on the quantities in the expressions (2.17)-(2.18), there may be real values of the parameters 'δ' and 'a' such that $\beta = 0$. Choosing the latter values for 'δ' and 'a' may reinforce the conclusions of item d) in Theorem 2.1.

3 Conclusions

We have given theoretical results for a class of preconditioners, which are parameter dependent. The preconditioners can be built by using any Krylov subspace method for the symmetric linear system (2.1), provided that the general conditions (2.2)-(2.3) in Assumption 2.1 are satisfied. We will give evidence in the companion paper [10] that in several real problems, a few iterations of the Krylov subspace method adopted may suffice to compute effective preconditioners. In particular, in many problems using a relatively small value of the index h, in Assumption 2.1, we can capture a significant information on the system matrix A. In order to clarify more carefully the latter statement, consider the eigenvectors $\{\nu_1, \ldots, \nu_n\}$ of matrix A in (2.1), and suppose the eigenvectors $\{\nu_{\ell_1}, \ldots, \nu_{\ell_m}\}$, with $\{\nu_{\ell_1}, \ldots, \nu_{\ell_m}\} \subseteq \{\nu_1, \ldots, \nu_n\}$, correspond to large eigenvalues of A (as often happens). In case the Krylov subspace method adopted to solve (2.1) generates directions which span the subspace $\{\nu_{\ell_1}, \ldots, \nu_{\ell_m}\}$, then $M_h^\sharp(a, \delta, D)$ will be likely effective as a class of preconditioners.

On this guideline our proposal seems tailored also for those cases where a sequence of linear systems of the form

$$A_k x = b_k, \qquad k = 1, 2, \ldots$$

requires a solution (e.g., see [14, 5] for details), where A_k slightly changes with the index k. In the latter case, the preconditioner $M_h^\sharp(a, \delta, D)$ in (2.6)-(2.7) can be computed applying the Krylov subspace method to the first linear system $A_1 x = b_1$. Then, $M_h^\sharp(a, \delta, D)$ can be used to efficiently solve $A_k x = b_k$, with $k = 2, 3, \ldots$.

Finally, the class of preconditioners in this paper seems a promising tool also for the solution of linear systems in financial frameworks. In particular, we want to focus on symmetric linear systems arising when we impose KKT conditions in portfolio selection problems, with a large number of titles in the portfolio, along with linear equality constraints (see also [2]).

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