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Polynomial acceleration of iterative schemes associated with subproper splittings

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Abstract: A subproper splitting of a matrix A is a decomposition $A=B-C$ such that the kernel of A includes that of B while the range of B includes that of A. Our purpose in the present work is to extend the convergence analysis of polynomial acceleration to the case of iterative schemes associated with subproper splittings, in the case of Hermitian matrices and consistent systems. Briefly stated, our conclusions show that the regular theory extends to the subproper case provided that "convergence to the solution of $Ax=b$" is understood as "convergence to a solution of $Ax=b$" while $\sigma(B^{-1}A)$ is understood as $\sigma(B^+A)\backslash\{0\}$ where B^+ is the Moore–Penrose inverse of B.

Keywords: Iterative methods for linear systems, acceleration of convergence, conditioning.

1. Introduction and notation

Let A be an Hermitian positive semidefinite $n\times n$ matrix and consider the possibly singular but consistent linear system

$$Ax=b \tag{1.1}$$

with $b\in R(A)$ (see below for notation).

We consider here iterative schemes based on a given splitting

$$A=B-C \tag{1.2}$$

(or "preconditioning"; B is called the preconditioning matrix) where B is an Hermitian positive semidefinite $n\times n$ matrix such that

$$N(B)\subset N(A) \tag{1.3}$$

which particularizes to Hermitian matrices the notion of subproper splitting introduced by Neumann in [16]. We are concerned here with polynomially accelerated iterative methods for solving (1.1), i.e. described by the following scheme

$$\begin{aligned}
&x_0=v_0\in S,\\
&Bv_{k+1}=Cv_k+b \quad \text{with } v_{k+1}\in S,\\
&x_{k+1}=\sum_{i=0}^{k+1}\alpha_{k+1}^i v_i, \quad k=0,1,2,\ldots
\end{aligned} \tag{1.4}$$

where S denotes a subspace of $\mathbb{C}^n$ complementary to $N(B)$ and where the coefficients α_{k+1}^i satisfy the relations

$$\sum_{i=0}^{k+1} \alpha_{k+1}^i = 1 \quad \text{for } k = 0, 1, 2, \dots . \tag{1.5}$$

It should be noticed that the linear system $Bv_{k+1} = Cv_k + b$ to be solved at each step is consistent (because (1.3) together with Hermitian symmetry implies that $R(A) \subset R(B)$ and $R(C) \subset R(B)$) and that it has a unique solution in S; the sequences (v_k) and (x_k) are therefore uniquely determined by v_0; in particular, if v_0 is a solution of (1.1), then $v_k = v_0$ for all k whence $x_k = v_0$ for all k by virtue of (1.5).

On the other hand, if the sequence (x_k) converges to a solution of (1.1), then, unless $N(B) = N(A)$, the latter will depend on v_0 (in practice, it will further depend on the rounding errors); it is therefore of interest to also consider the following more involved but more reliable scheme

$$\begin{aligned} &x_0 = v_0 \in T, \\ &Bw_{k+1} = Cv_k + b \quad \text{with } w_{k+1} \in S, \\ &v_{k+1} = P_{T,N(A)} w_{k+1}, \\ &x_{k+1} = \sum_{i=0}^{k+1} \alpha_{k+1}^i v_i, \quad k = 0, 1, 2, \dots \end{aligned} \tag{1.6}$$

where T denotes some subspace of $\mathbb{C}^n$ complementary to $N(A)$.

It will be seen that the convergence properties of the sequence (x_k) are identical for both processes (1.4) and (1.6) and further, independent of the choice of S.

Defining the polynomial

$$p_k(z) = \sum_{i=0}^{k} \alpha_k^i z^i \tag{1.7}$$

we have by (1.5) that

$$p_k(1) = 1 \tag{1.8}$$

whence it is seen that each one of the methods considered here is entirely characterized by a particular choice of a family of polynomials $p_k(z)$ of degree k such that $p_k(1) = 1$.

Basic unaccelerated iterative methods are included as the particular case determined by the family $p_k(z) = z^k$; the convergence properties of the latter methods have been investigated in the singular case (and in the more general setting of rectangular matrices) with regular preconditioning in [12,18] a.o. and with singular preconditioning in [6–8,10,13,16] (see also [17] for a survey).

To the author's knowledge, polynomial acceleration has received little attention in the singular case with regular preconditioning (cf. [2] for the conjugate gradient method and [15] for the method of steepest descent) and no attention at all with singular preconditioning and it is our purpose to fill this gap. Our analysis, which closely follows that of the regular case (cf. [3,4,11,19]) requires the use of generalized inverses whose needed properties will be recalled in the next section.

Spectral properties of possibly singular pencils of matrices are considered in Section 3.

Convergence results are developed in Sections 4 and 5. Section 6 contains our concluding remarks.

Notation

All vectors belong to $\mathbb{C}^n$, the n-dimensional complex space with euclidean scalar product denoted (x, y); all subspaces are subspaces of $\mathbb{C}^n$; all matrices are $n \times n$ complex matrices.

The symbols A^*, $A^{(1)}$, A^+, $N(A)$, $R(A)$, $\sigma(A)$ and $\|A\|$ denote respectively the adjoint, any $\{1\}$-inverse, the Moore–Penrose inverse, the null space, the range, the spectrum and the spectral norm of the matrix A.

By $P_{M,L}$ we denote the projector with null space L and range M (this notation implying that L and M are complementary subspaces).

If A is an $n \times n$ matrix and T a subspace of $\mathbb{C}^n$, we denote by A/T the linear operator in $\mathbb{C}^n$ defined as the restriction of A to T.

If A is an hermitian positive semidefinite matrix, we say that x and y are A-orthogonal if $(x, Ay) = 0$.

2. Generalized inverses

Needed properties of generalized inverses are briefly summarized in the present section, in the particular case of square matrices; we refer to [1] or [5] for a more detailed exposition.

We first recall that a $\{1\}$-inverse of an $n \times n$ matrix A is any $n \times n$ matrix X such that

$$AXA = A$$

or, equivalently, such that

$$AX/R(A) = I/R(A),$$

whence it follows that:

Theorem 2.1. *If A is an $n \times n$ matrix and if T is a subspace of $\mathbb{C}^n$ complementary to $N(A)$, then the unique solution of the consistent system*

$$Ax = y \quad \text{with } y \in R(A)$$

such that $x \in T$ is given by

$$x = P_{T,N(A)} A^{(1)} y$$

where $A^{(1)}$ denotes any $\{1\}$-inverse of A.

We next recall that the Moore–Penrose inverse, denoted A^+, of an $n \times n$ matrix A may be defined as its $\{1\}$-inverse such that

$$AA^+ = P_{R(A),R(A)^\perp}, \qquad A^+A = P_{N(A)^\perp,N(A)};$$

it exists, it is unique and it satisfies the following properties:

(1) $N(A^+) = R(A)^\perp$, $R(A^+) = N(A)^\perp$;

(2) for any $\{1\}$-inverse $A^{(1)}$ of A : $A^+ = P_{N(A)^\perp,N(A)} A^{(1)} P_{R(A),R(A)^\perp}$;

(3) $(A^+)^+ = A$;

(4) $(A^+)^* = (A^*)^+$;

(5) $(AB)^+ = B_1^+ A_1^+$, where $B_1 = A^+AB$ and $A_1 = AB_1B_1^+$; in particular, $(A^*A)^+ = A^+(A^*)^+$;

(6) if A is Hermitian, A^+ is Hermitian too, $N(A^+) = N(A) = R(A)^\perp = R(A^+)^\perp$, $AA^+ = A^+A + P_{R(A),N(A)}$ and A^+ may be characterized by its eigenvectors and eigenvalues which are such that

$$A^+x = \lambda^+x \quad \Leftrightarrow \quad Ax = \lambda x$$

with

$$\lambda^+ = \begin{cases} \lambda^{-1} & \text{if } \lambda \neq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{2.1}$$

3. Spectral analysis of pencils of matrices

We consider here pencils of matrices $A - \nu B$ where A and B are Hermitian positive semidefinite and such that $N(B) \subset N(A)$. It follows from these assumptions that $N(B)$ and $R(B) = N(B)^\perp$ are invariant subspaces of $A - \nu B$ and that the equation

$$Az = \nu Bz \tag{3.1}$$

is satisfied for all ν when $z \in N(B)$ showing that the spectral analysis of $A - \nu B$ reduces to that of its restriction to $N(B)^\perp$, which is a regular pencil because the restriction of B to $N(B)^\perp$ is positive definite on $N(B)^\perp$; further, it is readily seen from $N(B) \subset N(A)$ and $B^+B = P_{N(B)^\perp, N(B)}$ that $N(B)$ and $N(B)^\perp$ are also invariant subspaces of B^+A and that the relations

$$Az = \nu Bz, \quad z \in N(B)^\perp, \tag{3.2}$$

are equivalent to

$$B^+Az = \nu z, \quad z \in N(B)^\perp, \tag{3.3}$$

while $N(B^+A) \supset N(B)$, showing that the spectral analysis of $A - \nu B$ also reduces to that of B^+A.

These remarks lead us to the following result where eigenvectors of $A - \nu B$ for which (3.1) reduces to an identity (i.e. all vectors belonging to $N(B)$) are called trivial eigenvectors.

Theorem 3.1. *Let A and B be Hermitian positive semidefinite $n \times n$ matrices such that $N(B) \subset N(A)$. Then*:

(1) *the pencil $A - \nu B$ and the matrix B^+A have the same eigenvectors in $N(B)^\perp$;*

(2) *the trivial eigenvectors of $A - \nu B$ belong to $N(B^+A)$, i.e. are eigenvectors of B^+A associated with the eigenvalue* 0;

(3) *the nontrivial eigenvectors of $A - \nu B$ span $N(B)^\perp$ and we can choose among them a B-orthonormal basis of $N(B)^\perp$; they are associated, as eigenvectors of B^+A, to the same eigenvalues, all of which are nonnegative;*

(4) *the nontrivial eigenvectors of $A - \nu B$ associated with positive eigenvalues span the subspace V of $N(B)^\perp$ defined by*

$$V = \left\{ v \in N(B)^\perp;\ (v,\ Bu) = 0 \text{ for all } u \in N(A) \cap N(B)^\perp \right\};$$

V is complementary to $N(A)$ in $\mathbb{C}^n$ and we can choose among these eigenvectors a simultaneously B-orthonormal and A-orthogonal basis of V; therefore $N(B^+A) = N(A)$ and $R(B^+A) = V$;

(5) *if $\nu_{\min}$ and $\nu_{\max}$ denote respectively the smallest and largest positive eigenvalue of $A-\nu B$ associated with nontrivial eigenvectors, we have that*

$$\nu_{\min}=\min_{\substack{\nu\in\sigma(B^+A)\\ \nu\neq 0}}(\nu)=\min_{\substack{z\in V\\ z\neq 0}}\frac{(z,\ Az)}{(z,\ Bz)}\geqslant\min_{\substack{z\in S\\ z\neq 0}}\frac{(z,\ Az)}{(z,\ Bz)}\tag{3.4}$$

where S denotes any subspace of $\mathbb{C}^n$ complementary to $N(A)$ and

$$\nu_{\max}=\max_{\nu\in\sigma(B^+A)}(\nu)=\max_{\substack{z\in N(B)^{\perp}\\ z\neq 0}}\frac{(z,\ Az)}{(z,\ Bz)}=\max_{z\notin N(B)}\frac{(z,\ Az)}{(z,\ Bz)}.\tag{3.5}$$

Proof. (1) and (2) follow from the remarks above; (3), (4) and (5) follow from the same remarks and from the theory of regular pencils (cf. [9]) applied to the restriction of $A-\nu B$ to $N(B)^{\perp}$.

In particular, $N(A)\cap N(B)^{\perp}$ is the eigenspace of the latter pencil associated with the eigenvalue 0 while V is the subspace of $N(B)^{\perp}$ spanned by its eigenvectors associated with positive eigenvalues because V is the B-orthogonal complement of $N(A)\cap N(B)^{\perp}$ in $N(B)^{\perp}$; V is complementary to $N(A)$ in $\mathbb{C}^n$ because

$$N(B)^{\perp}=\left(N(A)\cap N(B)^{\perp}\right)\oplus V$$

while

$$N(A)=N(B)\oplus\left(N(A)\cap N(B)^{\perp}\right)$$

The only relation not covered by the classical theory of regular pencils is the inequality sub (3.4) which we now proceed to prove. For this purpose, it is sufficient to show that, for any $z\in V$, $z\neq 0$, we have

$$(z,\ Az)/(z,\ Bz)\geqslant(z',\ Az')/(z',\ Bz')\tag{3.6}$$

where $z'=P_{S,N(A)}z$; since $z'-z\in N(A)$ by definition of z', we have

$$(z',\ Az')=(z',\ Az)=(Az',\ z)=(Az,\ z)=(z,\ Az);\tag{3.7}$$

on the other hand,

$$(z',\ Bz')=(z,\ Bz)+2\,\mathrm{Re}[(z,\ B(z'-z))]+(z'-z,\ B(z'-z)),$$

but $z'-z\in N(A)=N(B)\oplus(N(A)\cap N(B)^{\perp})$ showing that $z'-z=z_1+z_2$ with $z_1\in N(B)$ and $z_2\in N(A)\cap N(B)^{\perp}$, whence

$$(z,\ B(z'-z))=(z,\ Bz_2)=0,$$

since V is B-orthogonal to $N(A)\cap N(B)^{\perp}$ in $N(B)^{\perp}$; therefore

$$(z',\ Bz')\geqslant(z,\ Bz)\tag{3.8}$$

which, together with (3.7), entails (3.6). □

Remark. We note here for later use that it follows from this analysis that V may also be defined as

$$V=\left\{v\in N(B)^{\perp};\ (v,\ Bu)=0\text{ for all }u\in N(A)\right\}\tag{3.9}$$

the latter relation also entails that A/V and B/V are both bijections from V onto $R(A)$, with $B^+/R(A)=(B/V)^{-1}$.

4. Polynomially accelerated iterative methods

We now return to the consideration of polynomially accelerated iterative methods for solving

$$Ax = b \quad \text{with } b \in R(A) \tag{4.1}$$

based on a given splitting $A = B - C$ where A and B are Hermitian positive semidefinite $n \times n$ matrices such that $N(B) \subset N(A)$.

We first observe that both methods described in Section 1 (cf. (1.4) and (1.6)) are particular cases of

$$x_0 = v_0 \in R(Q), \qquad v_{k+1} = QB^+(Cv_k + b),$$
$$x_{k+1} = \sum_{i=0}^{k+1} \alpha_{k+1}^i v_i, \quad k = 0, 1, 2, \ldots \tag{4.2}$$

where Q is some given projector such that

$$N(B) \subset N(Q) \subset N(A). \tag{4.3}$$

It follows indeed from Theorem 2.1 that

$$v_{k+1} = P_{S,N(B)} B^+(Cv_k + b) \tag{4.4}$$

when (1.4) is used while

$$v_{k+1} = P_{T,N(A)} P_{S,N(B)} B^+(Cv_k + b) = P_{T,N(A)} B^+(Cv_k + b) \tag{4.5}$$

when (1.6) is used; (4.2) is thus a more general scheme and it is the formulation that will be used from now on.

We next develop a few relations that will be useful both for the convergence analysis of the iterative scheme (4.2) and for its practical implementation. First, since $R(I - Q) = N(Q) \subset N(A)$, we have that $A(I - Q) = 0$, i.e.

$$AQ = A \tag{4.6}$$

whence, for any positive integer k,

$$(QB^+A)^k = Q(B^+A)^k \tag{4.7}$$

while, for any nonnegative integer k,

$$(QB^+A)^k Q = Q(B^+A)^k; \tag{4.8}$$

thus, for any polynomial $p(z)$,

$$p(QB^+A)Q = Qp(B^+A). \tag{4.9}$$

Next, because $R(I - B^+B) = N(B^+B) = N(B) \subset N(Q)$, we have that $Q(I - B^+B) = 0$, i.e.

$$QB^+B = Q \tag{4.10}$$

and it follows from the latter relation that the iterative scheme (4.2) is equivalent to

$$x_0 = v_0 \in R(Q), \qquad v_{k+1} = v_k + QB^+(b - Av_k),$$
$$x_{k+1} = \sum_{i=0}^{k+1} \alpha_{k+1}^i v_i, \quad k = 0, 1, 2, \ldots \tag{4.11}$$

a formulation that should be preferred in those applications where C is less sparse than A.

Further, letting $V = R(B^+A)$ (which is complementary to $N(B^+A) = N(A)$: cf. Section 3) and $\tilde{Q} = P_{V,N(A)}$, it follows from $R(I-Q) = N(Q) \subset N(A) = N(\tilde{Q})$ that $\tilde{Q}(I-Q) = 0$, i.e.

$$\tilde{Q}Q = \tilde{Q} \tag{4.12}$$

while, by the definition of $\tilde{Q}$,

$$\tilde{Q}B^+A = B^+A\tilde{Q} = B^+A, \tag{4.13}$$

$$(I-\tilde{Q})B^+A = B^+A(I-\tilde{Q}) = 0, \tag{4.14}$$

whence, for any polynomial $p(z)$,

$$p(B^+A)\tilde{Q} = \tilde{Q}p(B^+A), \tag{4.15}$$

$$p(B^+A)(I-\tilde{Q}) = p(0)(I-\tilde{Q}) = (I-\tilde{Q})p(B^+A). \tag{4.16}$$

Finally, it follows from (4.6) that if x is a solution to (4.1), so is Qx and, introducing $b = AQx$ in (4.11)

$$v_{k+1} - Qx = (I - QB^+A)(v_k - Qx)$$

whence by induction, for any nonnegative integer k,

$$v_k - Qx = (I - QB^+A)^k(v_0 - Qx)$$

and by (4.9), since $v_0 \in R(Q)$,

$$v_k - Qx = Q(I - B^+A)^k(v_0 - Qx). \tag{4.17}$$

Therefore, setting

$$\epsilon_k = x_k - Qx, \tag{4.18}$$

we have

$$\epsilon_k = Qp_k(I - B^+A)\epsilon_0 \tag{4.19}$$

where $p_k(z)$ denotes the polynomial of degree k defined by (1.7).

We shall now analyse the convergence of the iterative scheme (4.2); for this purpose, let $(\tilde{x}_k)$ denote the sequence generated by the following particular case of (4.2)–(4.11) (where $\tilde{Q}$ is choosen as projector):

$$\tilde{x}_0 = \tilde{v}_0 \in R(\tilde{Q}) = V,$$

$$\tilde{v}_{k+1} = B^+(C\tilde{v}_k + b) = \tilde{v}_k + B^+(b - A\tilde{v}_k).$$

$$\tilde{x}_{k+1} = \sum_{i=0}^{k+1} \alpha_{k+1}^i \tilde{v}_i, \quad k = 0, 1, 2, \dots . \tag{4.20}$$

We have then the following lemma.

Lemma 4.1. *Let* (x_k) *denote the sequence generated by* (4.2) (*or* (4.11)) *with given* x_0 *and let* $(\tilde{x}_k)$ *denote the sequence generated by* (4.20) *with* $\tilde{x}_0 = \tilde{Q}x_0$; *let* $|\cdot|$ *be any seminorm on* $\mathbb{C}^n$ *whose kernel is* $N(A)$ (*i.e. such that* $|u| = 0$ *if and only if* $u \in N(A)$); *then the following relations hold*:

$$\tilde{x}_k = \tilde{Q}x_k, \tag{4.21}$$

$$x_k = Q\tilde{x}_k + Q(I - \tilde{Q})x_0; \tag{4.22}$$

and the following propositions are equivalent:

(1) (x_k) *is convergent;*
(2) $(\tilde{x}_k)$ *is convergent;*
(3) $\exists s \in \mathbb{C}^n$ *such that* $|x_k - s| \to 0$ *for* $k \to \infty$;
(4) $\exists \tilde{s} \in V$ *such that* $|\tilde{x}_k - \tilde{s}| \to 0$ *for* $k \to \infty$.

Proof. Let x be a solution to (4.1) and $\tilde{x} = \tilde{Q}x$; define $\epsilon_k = x_k - Qx$ and $\tilde{\epsilon}_k = \tilde{x}_k - \tilde{Q}x$; it follows from (4.19), (4.15), (4.16), (4.12) and (1.8) that

$$\begin{aligned} x_k = \epsilon_k + Qx &= Qp_k(I - B^+A)\epsilon_0 + Qx \\ &= Qp_k(I - B^+A)\big(\tilde{Q}\epsilon_0 + (I - \tilde{Q})\epsilon_0\big) + Q\big(\tilde{Q}x + (I - \tilde{Q})x\big) \\ &= Q\tilde{Q}p_k(I - B^+A)\epsilon_0 + Q\tilde{x} + Q(I - \tilde{Q})(\epsilon_0 + x) \\ &= Q(\tilde{\epsilon}_k + \tilde{x}) + Q(I - \tilde{Q})(\epsilon_0 + Qx) \end{aligned}$$

whence (4.22); on the other hand, applying $\tilde{Q}$ on both sides of (4.22) we obtain (4.21), since $\tilde{Q}Q = \tilde{Q}$ and $\tilde{x}_k \in R(\tilde{Q})$.

Now, (1) $\Leftrightarrow$ (2) follows from (4.21), (4.22); further (2) $\Leftrightarrow$ (4) because $|\cdot|$ is a norm on V while (3) $\Leftrightarrow$ (4) because, letting $\tilde{s} = \tilde{Q}s$,

$$|x_k - s| = \big|\tilde{Q}(x_k - s) + (I - \tilde{Q})(x_k - s)\big| = |\tilde{x}_k - \tilde{s}| \tag{4.23}$$

since $R(I - \tilde{Q}) = N(\tilde{Q}) = N(A)$ which is the kernel of $|\cdot|$. □

We can now state our main convergence result:

Theorem 4.1. *Let A and B be Hermitian positive semi-definite $n \times n$ matrices such that $N(B) \subset N(A)$ and let $V = R(B^+A)$; let x_k be a sequence generated by the iterative scheme* (4.2) (*or equivalently* (4.11)) *where Q is a projector such that $N(B) \subset N(Q) \subset N(A)$ and where the polynomials*

$$p_k(z) = \sum_{i=0}^{k} \alpha_k^i z^i$$

satisfy $p_k(1) = 1$; let $\tilde{Q} = P_{V,N(A)}$ and let $\tilde{x}_k$ be a sequence generated by the iterative scheme (4.20); *let $|\cdot|$ be any seminorm on $\mathbb{C}^n$ whose kernel is $N(A)$; then the following propositions are equivalent:*

(1) $\forall x_0 : x_k$ *converges to some solution to* $Ax = b$;
(2) $\forall \tilde{x}_0 : \tilde{x}_k$ *converges to the solution* $\tilde{x} \in V$ *to* $Ax = b$;
(3) *for any solution x to $Ax = b$, and for any initial approximation x_0, $|x_k - x| \to 0$ for $k \to \infty$;*
(4) *for any initial approximation $\tilde{x}_0 \in V$, $|\tilde{x}_k - \tilde{x}| \to 0$ for $k \to \infty$, where $\tilde{x}$ denotes the unique solution to $Ax = b$ in V;*
(5) $p_k(I - B^+A)\tilde{Q} \to 0$ *for* $k \to \infty$;
(6) $\forall \nu \in \sigma(B^+A)\setminus\{0\} : p_k(1 - \nu) \to 0$ *for* $k \to \infty$;
(7) $M_k = \max_{\nu \in \sigma(B^+A)\setminus\{0\}} |p_k(1 - \nu)| \to 0$ *for* $k \to \infty$.

Proof. (1) $\Leftrightarrow$ (2) follows from Lemma 4.1; further (1) $\Leftrightarrow$ (3) since $|\cdot|$ is a seminorm on $\mathbb{C}^n$ with $N(A)$ as kernel; (2) $\Leftrightarrow$ (4) because $|\cdot|$ is a norm on V; (2) $\Leftrightarrow$ (5) follows from (4.19) in the particular case where $Q = \tilde{Q}$; (5) $\Leftrightarrow$ (6) follows from Theorem 3.1; (6) is obviously equivalent to (7). □

Incidentally, (4.22) shows that if x_k converges, it converges to $Q\tilde{x} + Q(I - \tilde{Q})x_0$ (which solves (4.1) if and only if x solves (4.1)) where $\tilde{x}$ is the limit of $\tilde{x}_k$ with $\tilde{x}_0 = \tilde{Q}x_0$.

Further, letting A_0, B_0 and C_0 denote the restrictions of A, B and C to V, it is readily seen from the remarks at the end of Section 3 that $\tilde{x}_k$ is identical to the sequence generated by the polynomial scheme associated with $p_k(z)$ and applied to the regular system

$$A_0 x = b \tag{4.24}$$

with regular preconditioning matrix B_0. With (4.23), the latter remark also shows that the convergence rate of anyone of the present schemes does not differ from that of the corresponding regular scheme applied to the regular system (4.24) with regular preconditioning matrix B_0, when estimated by a seminorm on $\mathbb{C}^n$ whose kernel is $N(A)$; using the seminorm $|\cdot|_A$ defined by

$$|u|_A = \sqrt{(u, Au)} \tag{4.25}$$

we have in particular the following theorem.

Theorem 4.2. *Under the same general assumptions as in Theorem* 4.1, *with* $\tilde{x}_0 = \tilde{Q}x_0$, *we have that*

$$|x_k - x|_A = |\tilde{x}_k - \tilde{x}|_A \leqslant M_k |\tilde{x}_0 - \tilde{x}|_A = M_k |x_0 - x|_A \tag{4.26}$$

where x *denotes any solution to* $Ax = b$, $\tilde{x} = Qx$ *and*

$$M_k = \max_{\nu \in \sigma(B^+A)\setminus\{0\}} |p_k(1-\nu)|. \tag{4.27}$$

Proof. It follows from the proof of Lemma 4.1 (cf. (4.23)) that

$$|x_k - x|_A = |\tilde{x}_k - \tilde{x}|_A;$$

further, from (4.19) in the case where $Q = \tilde{Q}$,

$$\tilde{x}_k - \tilde{x} = p_k(I - B^+A)(\tilde{x}_0 - \tilde{x})$$

or since $p_k(I - B^+A)/V = p_k(I - B_0^{-1}A_0)$, where $A_0 = A/V$ and $B_0 = B/V$,

$$|x_k - \tilde{x}|_A \leqslant \left|p_k\left(I - B_0^{-1}A_0\right)\right|_A |\tilde{x}_0 - \tilde{x}|$$

where

$$\left|p_k\left(I - B_0^{-1}A_0\right)\right|_A = \sup_{\substack{u \in V \\ u \neq 0}} \frac{\left|p_k\left(I - B_0^{-1}A_0\right)u\right|_A}{|u|_A}$$

and it is readily checked (by expanding u in the eigenvectors of $B_0^{-1}A_0$, remembering that $\sigma(B_0^{-1}A_0) = \sigma(B^+A)\setminus\{0\}$) that

$$\left|p_k\left(I - B_0^{-1}A_0\right)\right|_A = M_k.$$

5. Practical schemes

Practical schemes avoiding the use of the (v_k) sequence are readily deduced from the error evolution formula (4.19). For that purpose, assume that the polynomials $p_k(z)$ defined by (1.7) satisfy a recurrence relation of the form

$$p_{k+1}(z) = (a_k z + b_k) p_k(z) - c_k p_{k-1}(z) \tag{5.1}$$

for $k \geqslant 0$ (with $c_0 = 0$); to satisfy the normalization condition (1.8), we must have $a_k + b_k - c_k = 1$ whence, eliminating b_k,

$$p_{k+1}(z) - p_k(z) = a_k(z-1) p_k(z) + c_k(p_k(z) - p_{k-1}(z)); \tag{5.2}$$

therefore, from (4.19) and $AQx = b$,

$$x_{k+1} - x_k = a_k Q B^+ (b - Ax_k) + c_k(x_k - x_{k-1}) \tag{5.3}$$

or equivalently (setting $\delta_k = (x_{k+1} - x_k)/a_k$ and $d_k = c_k a_{k-1}/a_k$)

$$\delta_k = QB^+(b - Ax_k) + d_k \delta_{k-1}, \qquad x_{k+1} = x_k + a_k \delta_k \tag{5.4a,b}$$

for all $k \geqslant 0$ (with $c_0 = d_0 = 0$). Clearly, the formula (5.3) or (5.4) or variants of these are much better suited for practical implementation than the schemes considered in Section 4.

A few examples are reviewed below; the following notation is used throughout

$$\nu_{\min} = \min_{\nu \in \sigma(B^+A) \setminus \{0\}} (\nu), \qquad \nu_{\max} = \max_{\nu \in \sigma(B^+A) \setminus \{0\}} (\nu); \tag{5.5}$$

on the other hand, the appropriate determination of the iteration parameters may require bounds on the latter values and we then let $a < b$ be positive numbers such that $\sigma(B^+A) \setminus \{0\} \subset [a, b]$.

5.1. First order schemes

First order schemes are obtained from the preceding formula's when $c_k = 0$ for all $k \geqslant 0$; we have then from (5.2)

$$p_{k+1}(z) = (1 - a_k + a_k z) p_k(z)$$

whence by induction

$$p_{k+1}(z) = \prod_{i=0}^{k} (1 - a_i + a_i z) \tag{5.6}$$

while the iteration scheme becomes

$$x_{k+1} = x_k + a_k Q B^+ (b - Ax_k) \tag{5.7}$$

or

$$\delta_k = QB^+(b - Ax_k), \qquad x_{k+1} = x_k + a_k \delta_k. \tag{5.8a,b}$$

The unaccelerated method

It is associated with $a_k = 1$ for all $k \geqslant 0$, hence with the polynomials $p_k(z) = z^k$; by (7) of Theorem 4.1, it is convergent if and only if

$$\nu_{\max} < 2 \tag{5.9}$$

which is the convergence criterion of subproper splittings (cf. [17]) in the particular case of Hermitian matrices. Further,

$$M_k = \lambda^k \tag{5.10}$$

where

$$\lambda = \max(|1 - \nu_{\min}|,\ |\nu_{\max} - 1|) \tag{5.11}$$

The extrapolation method

It is associated with $a_k = \tau$ for all $k \geqslant 0$, hence with the polynomials

$$p_k(z) = (1 - \tau + \tau z)^k; \tag{5.12}$$

by (7) of Theorem 4.1, it is convergent if and only if

$$0 < \tau < 2/\nu_{\max} \tag{5.13}$$

If $\sigma(B^+A)\setminus\{0\} \subset [a,\ b]$ with $0 < a < b$ and $\tau = 2/(a+b)$, it is convergent with

$$M_k \leqslant ((b-a)/(b+a))^k. \tag{5.14}$$

The steepest descent method

It is associated with the parameters a_k which minimize the A-seminorm of the error (among all schemes of the form (5.7)); since

$$|\epsilon_{k+1}|_A = |x_{k+1} - x|_A = |x_k + a_k\delta_k - x|_A$$

with $\delta_k = QB^+(b - Ax_k)$ and $Ax = b$, it is readily seen by equating $(\partial/\partial a_k)|\epsilon_{k+1}|_A^2$ to zero that

$$a_k = (\delta_k,\ b - Ax_k)/(\delta_k,\ A\delta_k). \tag{5.15}$$

Now, defining $\tilde{x}_k$ by (4.21) and letting $\tilde{\delta}_k = B^+(b - A\tilde{x}_k)$, we have, since $N(Q) \subset N(A)$ and $R(A) = N(A)^\perp$

$$(\delta_k,\ b - Ax_k)/(\delta_k,\ A\delta_k) = (\tilde{\delta}_k,\ b - A\tilde{x}_k)/(\tilde{\delta}_k,\ A\tilde{\delta}_k)$$

showing, together with Theorem 4.2 (4.26) that the convergence analysis of the method can be performed on the regular system (4.24). Therefore (cf. [3,4]), it is always convergent with

$$M_k = \left(\frac{\nu_{\max} - \nu_{\min}}{\nu_{\max} + \nu_{\min}}\right)^k. \tag{5.16}$$

The Chebyshev method (first order version)

Choosing

$$a_k = \frac{2}{b + a - (b-a)\cos \pi\omega_k} \tag{5.17}$$

where

$$\omega_k = (2k+1)/2m, \quad k = 0, 1, 2, \ldots, m-1, \tag{5.18}$$

and $\sigma(B^+A)\setminus\{0\} \subset [a,\ b]$ with $0 < a < b$, one has

$$p_m(z) = \frac{T_m\left(\dfrac{2}{b-a}(z-1) + \theta\right)}{T_m(\theta)} \tag{5.19}$$

where $\theta=(b+a)/(b-a)$ and where $T_m(z)$ denotes the mth degree Chebyshev polynomial of the first kind; at the mth iteration, this scheme realizes

$$M_m \leqslant \frac{1}{T_m(\theta)} \leqslant 2\left(\frac{\sqrt{b}-\sqrt{a}}{\sqrt{b}+\sqrt{a}}\right)^m. \tag{5.20}$$

Using these parameters cyclically one obtains after l cycles

$$M_{lm} \leqslant \left(\frac{1}{T_m(\theta)}\right)^l \leqslant 2^l\left(\frac{\sqrt{b}-\sqrt{a}}{\sqrt{b}+\sqrt{a}}\right)^{lm}. \tag{5.21}$$

It should be mentioned here that, while the convergence properties of this method depend only on the set of parameters ω_k, its stability properties depend on the order in which these parameters are introduced (cf. [4] for example) and further that this method has been much improved by Lebedev and Finogenov [14] who produced infinite sequences of parameters ω_k such that

$$M_{k_i} \leqslant 1/T_{k_i}(\theta) \tag{5.22}$$

(exactly or approximately depending on the type of sequence) for some infinite subsequences k_i and for which the scheme (5.7) is stable.

5.2. Second order schemes

Orthogonal polynomials satisfy recurrence relations of the form (5.1) that may be used to generate second order schemes of the form (5.3) or (5.4) whenever $p_k(z)$ is a family of orthogonal polynomials.

The Chebyshev method (second order version)

Letting

$$p_k(z)=\frac{T_k\left(\frac{2}{b-a}(z-1)+\theta\right)}{T_k(\theta)} \tag{5.23}$$

where $\theta=(b+a)/(b-a)$, $\sigma(B^+A)\setminus\{0\}\subset[a,\ b]$ with $0<a<b$ and $T_m(z)$ denotes the mth degree Chebyshev polynomial of the first kind, we have that (5.2) holds with

$$a_0=2/(b+a),$$

$$a_k=\frac{4}{b-a}\frac{T_k(\theta)}{T_{k+1}(\theta)}, \qquad c_k=\frac{T_{k-1}(\theta)}{T_{k+1}(\theta)}, \quad k=1,\ 2,\dots\ . \tag{5.24}$$

The second order schemes (5.3) or (5.4) associated with these parameters is always (stable and) convergent with

$$M_k \leqslant \frac{1}{T_k(\theta)} \leqslant 2\left(\frac{\sqrt{b}-\sqrt{a}}{\sqrt{b}+\sqrt{a}}\right)^k \tag{5.25}$$

The conjugate gradient method

It is associated with the parameters a_k and d_k which minimize the A-seminorm of the error among all the schemes of the form (4.2) (or (4.11)). The classical analysis of the regular case applied to the system (4.24) with preconditioning matrix $B_0 = B/R(B^+A)$ leads us to (cf. [3,4])

$$a_k = \frac{(\tilde{\delta}_k,\ b - A\tilde{x}_k)}{(\tilde{\delta}_k,\ A\tilde{\delta}_k)}, \qquad d_k = \frac{(b - A\tilde{x}_k,\ B_0^{-1}(b - A\tilde{x}_k))}{(b - A\tilde{x}_{k-1},\ B_0^{-1}(b - A\tilde{x}_{k-1}))} \tag{5.26}$$

where $\tilde{x}_k$ is defined by (4.21) and $\tilde{\delta}_k = B_0^{-1}(b - A\tilde{x}_k)$. It is always convergent with

$$M_k \leqslant \frac{1}{T_k(\theta)} \leqslant 2\left(\frac{\sqrt{\nu_{\max}} - \sqrt{\nu_{\min}}}{\sqrt{\nu_{\max}} + \sqrt{\nu_{\min}}}\right)^k. \tag{5.27}$$

Now, since $B_0^{-1} = B^+/R(A)$, $A\tilde{x}_k = Ax_k$ for all k, $N(Q) \subset N(A)$ and $R(A) = N(A)^{\perp}$, (5.26) may equivalently be written

$$a_k = \frac{(\delta_k,\ b - Ax_k)}{(\delta_k,\ A\delta_k)}, \qquad d_k = \frac{(b - Ax_k,\ QB^+(b - Ax_k))}{(b - Ax_{k-1},\ QB^+(b - Ax_{k-1}))}, \tag{5.28}$$

which is easier to implement in the scheme (5.4).

6. Concluding remarks

The spectral condition number of a nonsingular $n \times n$ matrix A is defined as

$$\kappa(A) = \| A^{-1} \| \cdot \| A \|$$

reducing to

$$\kappa(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$$

when A is Hermitian positive definite, $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ denoting the smallest and largest eigenvalues of A; in the latter case, we also have

$$\kappa(F^{-1}AF^{*-1}) = \lambda_{\max}(F^{-1}AF^{*-1})/\lambda_{\min}(F^{-1}AF^{*-1})$$

where F is any nonsingular $n \times n$ matrix and therefore also

$$\kappa(F^{-1}AF^{*-1}) = \lambda_{\max}(B^{-1}A)/\lambda_{\min}(B^{-1}A)$$

with $B = FF^*$, a relation which is often (abusively) written

$$\kappa(B^{-1}A) = \lambda_{\max}(B^{-1}A)/\lambda_{\min}(B^{-1}A).$$

Our results suggest to extend the latter definition to the singular case by setting

$$\kappa(B^+A) = \nu_{\max}/\nu_{\min}$$

when A and B are Hermitian positive semidefinite with $N(B) \subset N(A)$, $\nu_{\min}$ and $\nu_{\max}$ being defined by (5.5); here also, $\kappa(B^+A)$ should be understood as an abusive notation for $\kappa(F^+AF^{*+})$ with $B = FF^*$ (whence $B^+ = F^{*+}F^+$ by (5) of Section 2), the definition of $\kappa(A)$ being extended to the case of any $n \times n$ matrix A through

$$\kappa(A) = \| A^+ \| \cdot \| A \|.$$

With these definitions, our results show that, when expressed as functions of $\kappa(B^+A)$, the convergence rates of polynomially accelerated iterative schemes considered here do not depend on the regularity of the pencil.

To emphasize the relevance of these conclusions we notice here that, in view of the difficulties to find convergent splittings for singular systems, it has been suggested to give up iterative schemes in favour of direct or combined direct-iterative approaches to solve singular systems (cf. [17]); our conclusions suggest to try polynomial acceleration first.

By way of illustration, let $Ax = b$ (resp. $A_0x = b$) be the 5-point finite difference approximation to the Neumann (resp. Dirichlet) problem associated with the Laplacian operator on the unit square in the x–y plane, using a uniform square mesh of mesh size $h = 1/N$ and let $D = \text{diag}(A)$ (resp. $D_0 = \text{diag}(A_0)$); then

$$\nu_{\min}(D^{-1}A) = \tfrac{1}{2}(1 - \cos \pi/N), \qquad \nu_{\max}(D^{-1}A) = 2,$$

$$\kappa(D^{-1}A) = \frac{4}{1 - \cos \pi/N} \simeq \frac{8N^2}{\pi^2},$$

while

$$\nu_{\min}(D_0^{-1}A) = 1 - \cos \pi/N,$$

$$\nu_{\max}(D_0^{-1}A) = 1 + \cos \pi/N,$$

$$\kappa(D_0^{-1}A_0) = \frac{1 + \cos \pi/N}{1 - \cos \pi/N} \simeq 4N^2/\pi^2,$$

showing that while the Jacobi method is not convergent in the singular case, polynomially accelerated Jacobi methods behave similarly to solve both problems. In other words, polynomially accelerated schemes, besides being faster, have a wider scope of application.

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