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Deflation and projection methods applied to symmetric positive semi-definite systems

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ABSTRACT

Linear systems with a singular symmetric positive semi-definite matrix appear frequently in practice. This usually does not lead to difficulties for CG methods as long as these systems are consistent. However, the construction of a preconditioner, especially the construction of two-level and multilevel methods, becomes more complicated, since singular coarse grid matrices or Galerkin matrices may occur. Here we continue the work started in [21,22] where deflation is used for some special singular coefficient matrices. Here we show that deflation and other projection-type preconditioners can be applied to arbitrary singular problems without any difficulties. In each of these methods, a two-level preconditioner is involved where coarse-grid systems based on a singular Galerkin matrix should be solved. We prove that each projection operator consisting of a singular Galerkin matrix can be written as an operator with a nonsingular Galerkin matrix. Therefore many results that hold for nonsingular

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Galerkin matrices are also valid for problems with singular Galerkin matrices.

1. Introduction

The conjugate gradient (CG) method [6] is the method of choice for solving linear systems of the form

$$Ax = b, \quad A \in \mathbb{R}^{n\times n},$$

whose coefficient matrix, A, is sparse and symmetric positive semi-definite (SPSD). However, in order to speed up the convergence of CG, an efficient symmetric positive definite (SPD) preconditioner, M^{-1}, is needed. With a preconditioner, the system

$$M^{-1}Ax = M^{-1}b,$$

is then to be solved by CG. The preconditioner, M^{-1}, must be chosen such that $M^{-1}A$ has a more clustered spectrum or a smaller condition number than A. Furthermore, the system $My_2 = y_1$ must be cheap to solve relative to the improvement it provides in convergence rate. Nowadays, the design and analysis of preconditioners for CG is the main focus whenever a linear system with an SPSD coefficient matrix needs to be solved.

Stimulated by the numerical solution of PDEs and the problem of solving the resulting linear system, two-level or multi-level preconditioners have been developed successfully during the last decades. These preconditioners make use of the solution of smaller systems, which are also known as Galerkin systems or coarse-grid systems. In combination with traditional preconditioners, such as Jacobi and Gauss–Seidel, these preconditioners have become a powerful tool. Examples of these preconditioners are the geometric and algebraic multigrid methods (see, e.g., [25,27]) and domain decomposition methods with coarse-grid corrections, such as the BPS method [2,3] and the balancing Neumann–Neumann method [9–11]. In the same period, the so-called augmented Krylov-subspace methods were established [13]. These methods are also known as deflation-type methods [17,19].

At a first glance, all of the above described projection methods differ a lot in practice. However, from an abstract point of view, there are many common ingredients. Each of these methods use a projection of the form

$$P := I - AQ, \quad Q := ZE^{-1}Z^T, \quad E := Z^TAZ, \tag{1.1}$$

where we assume that $Z \in \mathbb{R}^{n\times r}$ is given such that E is nonsingular. In classical multilevel methods, Z is called a prolongation operator, while Z^T acts as a restriction operator. Moreover, E is known as the coarse-grid or Galerkin matrix. In the deflation methods, the matrix Z consists of deflation vectors and Z is called the deflation-subspace matrix. Finally, Q is known as the correction matrix.

In [14–16,23], a detailed abstract comparison of some of these projection or coarse-grid correction methods applied to an SPD coefficient matrix, A, and a full-rank matrix, Z, is presented. It has been shown that most of these methods are strongly related to each other. Some of these methods are even mathematically equivalent.

Linear systems with a singular symmetric positive semi-definite matrix appear frequently in practice, especially, in the numerical solutions of PDEs if Neumann boundary conditions are involved. Here, we consider arbitrary SPSD coefficient matrices and arbitrary restriction operators or deflation-subspace matrices. In this case, the coarse-grid matrix, E, might be singular. Hence, the projection (1.1) is no longer well-defined. Instead of using the inverse in (1.1), one needs to use the Moore–Penrose inverse (or an iterative method to solve the related coarse-grid system), so that we end up with the projection

$$P_+ := I - AQ_+, \quad Q_+ := ZE^+Z^T, \quad E := Z^TAZ. \tag{1.2}$$

In this paper, we show that there is another way to handle the singularity of the coarse grid matrix. We prove that for any SPSD coefficient matrix and deflation-subspace matrix there exists a reduced deflation-subspace matrix, called $Z_a \in \mathbb{R}^{n,t}$ with $t \leq r$, so that the resulting Galerkin matrix, $E_a := Z_a^TAZ_a$, is nonsingular, and the resulting correction matrix, $Q_a := Z_aE_a^{-1}Z_a^T$, is identical to the original correction matrix, Q_+. Thus surprisingly, using matrix Z_a that have fewer columns than the original matrix Z, one can avoid the singularity but the effect of the correction matrix stays the same.

However, in order to build the reduced deflation-subspace matrix Z_a, some spectral information is needed. We show that one can create another reduced deflation subspace matrix, Z_b, for which in general $Q_+ \neq Q_b$ with $Q_b := Z_bE_b^{-1}Z_b^T$ and $E_b = Z_b^TAZ_b$, but

$$P_+A = P_bA \tag{1.3}$$

holds, where $P_b := I - AQ_b$. Hence, from a theoretical point of view, singular coarse-grid systems can be avoided without losing the requested properties, such as spectral and approximation properties of the projections or subspace-correction matrices.

In the literature, various contributions have been made regarding the application of deflation to special singular coefficient matrices, see [21,22]. For this special case, some more information about A and E is known. In these papers, some variants of the deflation method for specific system matrices A arising in the numerical simulation of bubbly flow problems are discussed. These variants can deal with the singularity of the specific coefficient matrix. They are based on

1. A that is modified such that it is nonsingular;
2. the original Z in which the last column is omitted so that E becomes nonsingular;
3. Galerkin systems which are solved iteratively.

It can be proven for the specific matrices A that the above three variants are mathematically equivalent. However, there is a gap in the proof of [22, Thm. 4.3], where it was stated that the reduction of the last column of Z leads to a nonsingular new E. By proving more general theorems in this paper, we fill this gap.

The transformation from singular to nonsingular Galerkin matrices allows us further to establish a precious statement of the zero structure of the deflated system matrix. Moreover, we introduce variants of well-known deflation and projection preconditioners using the Moore–Penrose inverse. We establish spectral properties of these variants applied to singular matrices.

The paper is organized as follows. Some notation and preliminary results are given in Section 2. Section 3 is devoted to new theoretical results for the deflation methods. Subsequently, similar results are presented for other projection and coarse-grid correction methods in Section 4. Finally, the conclusions are given in Section 5. For numerical experiments based on the theory developed in this paper, we refer to [21–23].

2. Notation and preliminary results

In the following, we denote by $\lambda_i(C)$ the eigenvalues of a matrix C. If the eigenvalues are real, the set $\{\lambda_i(C)\}$ is ordered increasingly. By $\mathcal{N}(C)$ we denote the null space of C, while $\mathcal{R}(C)$ denotes the range of C. In addition, for two Hermitian matrices B and C, we write $B \succeq C$, if $B - C$ is positive semi-definite.

We start with Assumption 1 that holds throughout the paper without explicit mentioning.

Assumption 1. *Let $A \in \mathbb{R}^{n\times n}$ be an SPSD matrix, where the dimension of the null space of A is denoted by s, so that the dimension of the range of A is $n-s$, i.e., $\dim \mathcal{N}(A) = s$ and $\dim \mathcal{R}(A) = n - s$. Moreover, we suppose that $Z \in \mathbb{R}^{n,r}$ is given such that $\mathcal{R}(E) = t$ with $t \leq r$.*

Next, we list the following well-known result for singular matrices (see e.g.[1]).

Theorem 2.1. *Let $E \in \mathbb{R}^{r\times r}$ be given. Then, there exists an unique matrix, E^+, such that the following equations hold:*

$$\begin{cases} E^+EE^+ &= E^+; \\ EE^+E &= E; \\ (E^+E)^T &= E^+E; \\ (EE^+)^T &= EE^+. \end{cases} \tag{2.1}$$

E^+ is often called the pseudo-inverse or Moore–Penrose inverse of E.

Next, we mention well-known properties of the eigenvalues of Hermitian matrices.

Lemma 2.2. *Let $B, C \in \mathbb{C}^{n\times n}$ be Hermitian. For each $k = 1, 2, \dots, n$, we have*

$$\lambda_k(B) + \lambda_1(C) \leq \lambda_k(B + C) \leq \lambda_k(B) + \lambda_n(C).$$

From the above lemma, we easily obtain the next lemma.

Lemma 2.3. *If $B, C \in \mathbb{C}^{n\times n}$ are positive semi-definite with $B \succeq C$, then $\lambda_i(B) \geq \lambda_i(C)$ for all $i = 1, 2, \dots, n$.*

Moreover, we will use the following lemma in this paper.

Lemma 2.4. *Let $B, C \in \mathbb{C}^{n\times n}$ be Hermitian and suppose that C has rank at most r. Then,*

- $\lambda_k(B + C) \leq \lambda_{k+r}(B)$, $k = 1, 2, \dots, n - r$;
- $\lambda_k(B) \leq \lambda_{k+r}(B + C)$, $k = 1, 2, \dots, n - r$.

Lemmas 2.2, 2.3 and 2.4 can be found in, e.g., [5, Thm. 4.3.1, Cor. 7.7.4, Thm. 4.3.6], respectively.

Subsequently, we define the inertia of a Hermitian matrix.

Definition 2.5. Let $B \in \mathbb{C}^{n\times n}$ be a Hermitian matrix. The inertia of B is the ordered triple

$$i(B) := (i_+(B), i_-(B), i_0(B)),$$

where $i_+(B)$ is the number of positive eigenvalues of B, $i_-(B)$ is the number of negative eigenvalues of B, and $i_0(B)$ is the number of zero eigenvalues of B, all counting multiplicity.

Using the above definition, we obtain the following standard result.

Lemma 2.6. *Let $B \in \mathbb{C}^{n\times n}$ be a Hermitian matrix and let $S \in \mathbb{C}^{n\times n}$ be nonsingular. Then,*

$$i(B) = i(SBS^H).$$

Finally, we state the interlacing theorem for Hermitian matrices.

Lemma 2.7. *Let $B \in \mathbb{C}^{n\times n}$ be a Hermitian matrix and let $\widetilde{B}$ be a leading principal submatrix of B. Then,*

$$\lambda_i(B) \leq \lambda_i(\widetilde{B}) \leq \lambda_{i+1}(B),$$

for $i = 1, \dots, n - 1$.

Lemmas 2.6 and 2.7 can be found in, e.g., [5, Thms. 4.5.8 and 4.3.8], respectively.

3. Deflation methods

In this section, we present and analyze the deflation method for an SPSD coefficient matrix, A, but we start with reviewing the deflation method for a (nonsingular) SPD coefficient matrix, A.

3.1. Deflation method for a nonsingular coefficient matrix

The deflation technique has been exploited by several authors, among them are Nicolaides [17], Morgan [13], Kolotilina [7], and Saad, Yeung, Erhel, and Guyomarc'h [19], see also Padiy, Axelsson and Polman [18]. There are many different ways to describe the deflation technique. We prefer the following one.

As mentioned above, we define the deflation or projection matrix, $P \in \mathbb{R}^{n\times n}$, by (1.1), where $\mathcal{R}(Z)$ is the deflation subspace, and I is the identity matrix of appropriate size. Moreover, $E \in \mathbb{R}^{r\times r}$ is the invertible Galerkin matrix, and $Q \in \mathbb{R}^{n\times n}$ is the correction matrix.

If we assume that Z has rank r, then E is SPD. Since $x = (I - P^T)x + P^T x$ and because

$$(I - P^T)x = QAx = Qb \tag{3.1}$$

can be computed immediately, we only need to compute $P^T x$. In light of the identity $AP^T = PA$, we can solve the deflated system

$$PA\tilde{x} = Pb$$

by using CG, premultiply $\tilde{x}$ by P^T, and add it to (3.1).

The deflated system can also be solved by using an SPD preconditioner, M^{-1}, by solving

$$M^{-1}PA\tilde{x} = M^{-1}Pb,$$

using CG.

In the following, we list some properties and equalities that are often used to analyze deflation methods.

Lemma 3.1. *Let $A \in \mathbb{R}^{n\times n}$ be an SPD matrix, and let P, Q, Z be as defined in (1.1). Then, the following equalities hold:*

(a) $P = P^2$;
(b) $PA = AP^T$;

(c) $P^TZ = 0$, $P^TQ = 0$;
(d) $PAZ = 0$, $PAQ = 0$;
(e) $QA = I - P^T$, $QAZ = Z$, $QAQ = Q$;
(f) $Q^T = Q$.

Moreover, we have

$$\sigma(M^{-1}PA) = \{0, \dots 0, \delta_{r+1}, \dots, \delta_n\}, \quad \delta_i > 0, \quad i = r+1, \dots, n. \tag{3.2}$$

3.2. Deflation method for a singular coefficient matrix

We now consider the situation with an SPSD coefficient matrix, A. As in the nonsingular case, we assume that the preconditioning matrix, M^{-1}, is SPD. However, we allow arbitrary deflation-subspace matrices, i.e., Z does not necessarily have full rank. Then, we define the Galerkin matrix, E, the correction matrix, Q_+, and the deflation matrix, P_+, as in (1.2) It is not hard to see that some of the properties that hold for the nonsingular case are also valid for the singular case. However, it is important to note that some of these properties do not hold for the singular case. Both P and P_+ are projections, but they project onto and along different subspaces.

This will be further explained below.

Using the properties of the Moore–Penrose inverse of E (see Theorem 2.1), we obtain the following lemma, which states identities that are the same for the nonsingular case.

Lemma 3.2. *Let $A \in \mathbb{R}^{n\times n}$ be an SPSD matrix, and let P_+, Q_+, Z be as defined in (1.2). Then, the following equalities hold:*

(a) $P_+ = P_+^2$;
(b) $P_+A = AP_+^T$;
(c) $Q_+A = I - P_+^T$, $Q_+AZ = Z$, $Q_+AQ_+ = Q_+$;
(d) $Q_+^T = Q_+$.

Proof. We easily obtain

$$\begin{aligned} P_+^2 &= (I - AZE^+Z^T)^2 \\ &= I - 2AZE^+Z^T + AZE^+Z^TAZE^+Z^T \\ &= I - AZE^+Z^T \\ &= P_+. \end{aligned}$$

Thus, (a) holds. The other properties can be established in a similar way. □

However, in contrast to the case with a nonsingular matrix A, we have

$$\begin{cases} P_+^T Z &= Z - ZE^+E; \\ P_+AZ &= AZ - AZE^+E. \end{cases}$$

Both terms are generally not zero, i.e., (c) and (d) of Lemma 3.1 are not valid for the singular case. Instead, the following lemma holds.

Lemma 3.3. *Let $A \in \mathbb{R}^{n\times n}$ be an SPSD matrix, and let P_+, Q_+, Z be as defined in (1.2). Then, the following equalities hold:*

(a) $P_+^T Z E^+ = 0$;
(b) $P_+AZE^+ = 0$;
(c) $Z^T P_+ AZ = 0$.

Proof. For (a), we have

$$P_+^T Z E^+ = ZE^+ - ZE^+EE^+ = 0.$$

Similarly,

$$P_+AZE^+ = AZE^+ - AZE^+EE^+ = 0,$$

and

$$Z^T P_+ AZ = Z^T AZ - Z^T AZE^+E = 0.$$

Thus, (b) and (c) hold. □

Moreover, we have the following lemma.

Lemma 3.4. *Let $A \in \mathbb{R}^{n\times n}$ be an SPSD matrix, and let P_+ be as defined in (1.2). Then, P_+A is SPSD.*

Proof. Using Lemma 3.2, we obtain

$$P_+A = P_+^2 A = P_+AP_+^T.$$

Since A is SPSD, this implies that P_+A is SPSD. □

With the help of the above properties, a solution of the singular linear system, $Ax = b$, can be computed by using a technique similar to that described at the beginning of this section. We first solve the singular system

$$M^{-1}P_+A\tilde{x} = M^{-1}P_+b. \tag{3.3}$$

Then, $\widetilde{x}$ is multiplied by P_+^T and Q_+b is added. We obtain

$$A(P_+^T\tilde{x} + Q_+b) = P_+b + AQ_+b = b,$$

so $P_+^T\tilde{x} + Q_+b$ is a solution of the system $Ax = b$. Note that the solution of (3.3) is unique up to contributions of the null space of $M^{-1}P_+A$.

3.3. Theoretical properties

We consider the properties of the linear system (3.3). We start by considering the Galerkin matrix E and, thereafter, the correction matrix Q_+ and the projection matrix, P_+.

Proposition 3.5. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD. Let $Z \in \mathbb{R}^{n\times r}$ be given with $\operatorname{rank} Z = r$. Then, E is nonsingular if and only if $\mathcal{N}(A) \cap \mathcal{R}(Z) = \{0\}$ holds.*

Proof. Since E is symmetric, it is nonsingular if and only if $y^TEy > 0$ for all $y \neq 0$. But since, $\mathcal{N}(A) \cap \mathcal{R}(Z) = \{0\}$, all vectors $Zy \neq 0$ are not in $\mathcal{N}(A)$. Hence, $y^TEy = (Zy)^TA(Zy) > 0$. If E is nonsingular, then obviously $\mathcal{N}(A) \cap \mathcal{R}(Z) = \{0\}$ holds. □

Subsequently, we show that the original deflation matrix based on a singular Galerkin matrix can always be written as a deflation matrix with a nonsingular Galerkin matrix.

Theorem 3.6. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD. Let $Z \in \mathbb{R}^{n\times r}$ be given. Then, there is a matrix $Z_a \in \mathbb{R}^{n\times t}$ with $t \leq r$ and rank $(Z_a) = t$ such that $E_a := Z_a^TAZ_a$ is invertible and*

$$Q_+ = Q_a, \quad P_+ = P_a,$$

where $Q_a := Z_aE_a^{-1}Z_a^T$ and $P_a := I - AQ_a$.

Proof. First, observe that, for an orthogonal matrix $U \in \mathbb{R}^{r\times r}$, we have

$$ZU(U^TZ^TAZU)^+U^TZ^T = Z(Z^TAZ)^+Z^T = Q_+.$$

Next, since E is SPSD, there exists an orthogonal matrix $U \in \mathbb{R}^{r\times r}$ such that

$$U^TZ^TAZU = \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix},$$

where $D_1 \in \mathbb{R}^{t\times t}$ with $t \leq r$ is a nonsingular diagonal matrix. Now, let

$$U = [U_1,\ U_2], \quad U_1 \in \mathbb{R}^{r\times t}, \quad U_2 \in \mathbb{R}^{r\times(r-t)},$$

and $Z_a := ZU_1 \in \mathbb{R}^{r\times t}$.

Since

$$Z_a^T A Z_a = U_1^T Z^T A Z U_1 = D_1,$$

and by construction $D_1 \in \mathbb{R}^{t\times t}$ is a nonsingular matrix, Z_a must have full rank, t and $E_a = Z_a^T A Z_a = D_1$ is nonsingular. Then, we obtain

$$ZU = [ZU_1,\ ZU_2], \qquad (ZU)^T = \begin{bmatrix} U_1^T Z^T \\ U_2^T Z^T \end{bmatrix}.$$

Hence,

$$\begin{aligned} Q_+^T &= ZU(U^T Z^T A Z U)^+ U^T Z^T \\ &= ZU \left(\begin{bmatrix} U_1^T Z^T \\ U_2^T Z^T \end{bmatrix} A[ZU_1, ZU_2] \right)^+ U^T Z^T \\ &= [ZU_1, ZU_2] \begin{bmatrix} D_1^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} U_1^T Z^T \\ U_2^T Z^T \end{bmatrix} \\ &= ZU_1 D_1^{-1} U_1^T Z^T \\ &= ZU_1 (U_1^T Z^T A Z U_1)^{-1} U_1^T Z^T \\ &= Z_a (Z_a^T A Z_a)^{-1} Z_a^T. \end{aligned}$$

This implies that

$$Q_+ = Q_a, \quad P_+ = P_a,$$

which completes the proof. □

Theorem 3.6 shows that for each SPSD coefficient matrix, A, and each deflation-space matrix, Z, there exists a reduced deflation-space matrix, Z_a, such that $E_a := Z_a^T A Z_a$ is nonsingular and the projection P_+ is equal to another projection based on E_a. Moreover, Theorem 3.6 also provides a technique to construct the deflation-space matrix Z_a.

We will establish another way for the construction of Z_a, if some more properties of A and E are known. To do so, we slightly generalize a result that is given in [14].

Theorem 3.7. *Let A be SPSD. Let $Z, V \in \mathbb{R}^{n\times r}$ be full-rank matrices such that $E_Z := Z^T A Z$ and $E_V := V^T A V$ are nonsingular and $\mathcal{R}(Z) = \mathcal{R}(V)$. Then,*

$$Z E_Z^{-1} Z^T = V E_V^{-1} V^T.$$

Proof. The proof is the same as the proof of [14, Lemma 2.9], where the nonsingularity of A has not been used. $\square$

Following the proof of Theorem 3.6, the reduced deflation-space matrix, Z_a, is given by

$$Z_a = ZU_1.$$

Now, if we have a matrix W satisfying $\mathcal{R}(U_1) = \mathcal{R}(W)$, we obtain $\mathcal{R}(ZU_1) = \mathcal{R}(ZW)$ so that we can use Theorem 3.7 to get the reduced deflation space. Such a matrix W will be constructed in the next theorem.

Theorem 3.8. *Let A be SPSD. Let $Z \in \mathbb{R}^{n\times r}$ be given such that it satisfies* $\operatorname{rank}(Z^TAZ) = t$. *Moreover, let Q_+ and Q_a be as in Theorem 3.6. Let W consist of basis vectors of the orthogonal complement of $\mathcal{N}(E)$. Let $Z_s = ZW$, then*

$$Q_+ = Q_a = Q_s,$$

where $Q_s := Z_s E_s^{-1} Z_s^T$ and $E_s := Z_s^T A Z_s$.

Proof. Following the proof of Theorem 3.6, the reduced deflation-space matrix, Z_a is given by

$$Z_a = ZU_1.$$

If we have a matrix W satisfying $\mathcal{R}(U_1) = \mathcal{R}(W)$, we obtain $\mathcal{R}(ZU_1) = \mathcal{R}(ZW)$. As shown in the proof of Theorem 3.6, U_1 consists of the eigenvectors of E corresponding to the nonzero eigenvalues. But, since E is symmetric, these eigenvectors are orthogonal to the eigenvectors corresponding to the eigenvalue zero, i.e., the null space of A. Note that, by construction, $Z_a = ZU$ has full rank, i.e., $\operatorname{rank} Z_a = t$. Thus, if one knows the null space of E and one can construct a basis of the orthogonal complement, say W, then $U_1 = WT$ for a nonsingular matrix T. Hence,

$$\mathcal{R}(ZU_1) = \mathcal{R}(ZW).$$

Thus, using Theorem 3.7, ZW can also be used as a reduced deflation-space matrix, and we have the desired result. $\square$

In this section we gave several ways how to handle singular coarse grid systems without using the Moore–Penrose inverse explicitly. Of course one needs to know a basis of the orthogonal complement of $\mathcal{N}(E)$. We will use this construction in the next subsection for a special case, where such a basis can be constructured easily.

3.4. Theoretical properties for specific problems

Here, we discuss some properties of the deflation method for specific problems, namely the matrices resulting from the numerical solution of bubbly flow problems [22]. For more details about the bubbly flow problem see [21] and [22]. In this special case some more information about A and E is given. If $e_n \in \mathbb{R}^n$ denotes the all–one vector then the coefficient matrix A satisfy $Ae_n = 0$ and rank $A = n-1$. Moreover Z is chosen such that $Ze_r = e_n$ and rank $E = r - 1$. In this situation, Theorem 3.8 leads to a simple way to construct a reduced deflation space. Here we only need to remove an arbitrary column of Z.

Theorem 3.9. *For $l \geq 0$ let $e_l \in \mathbb{R}^l$ be the all–one vector. Let A be SPSD and $Z \in \mathbb{R}^{n\times r}$, $r \geq 2$, be given such that*

$$Ae_n = 0; \tag{3.4}$$

$$Ze_r = e_n; \tag{3.5}$$

$$\operatorname{rank} A = n - 1; \tag{3.6}$$

$$\operatorname{rank} E = r - 1. \tag{3.7}$$

Suppose that

$$Z = [z_1, \dots, z_r], \quad \widetilde{Z} = [z_1, \dots, z_{k-1}, z_{k+1}, \dots, z_r], \quad \textit{for some} \quad k \in \{1, \dots, r\}.$$

Moreover, we define

$$\widetilde{P} := I - A\widetilde{Q}, \quad \widetilde{Q} := \widetilde{Z}\widetilde{E}^{-1}\widetilde{Z}^T, \quad \widetilde{E} := \widetilde{Z}^T A\widetilde{Z}.$$

Then, $\widetilde{E}$ is nonsingular and the following equalities hold:

$$AQ_+A = A\widetilde{Q}A, \quad P_+A = \widetilde{P}A,$$

where Q_+ and P_+ are defined as in Eq. (1.2).

Proof. Since Eqs. (3.4) and (3.5) hold, we have $Ee_r = 0$ so that $\mathcal{N}(E) = \operatorname{span}\{e_r\}$.

Next, we choose a basis W of the orthogonal complement of $\mathcal{N}(E)$. We take the set of vectors $\{w_i \in \mathbb{R}^r : i = 1\dots, r, i \neq k\}$ given by

$$w_1 = \left[1, \frac{-1}{r-1}, \dots, \frac{-1}{r-1}\right]^T;$$

$$w_2 = \left[\frac{-1}{r-1}, 1, \frac{-1}{r-1}, \dots, \frac{-1}{r-1}\right]^T;$$

$$\vdots$$

$$w_r = \left[\frac{-1}{r-1}, \ldots, \frac{-1}{r-1}, 1\right]^T.$$

Eq. (3.5) gives us

$$z_1 = e_n - \sum_{j=2}^{r} z_j,$$

which can be written as

$$\frac{1}{r-1} z_1 = \frac{1}{r-1}\left(e_n - \sum_{j=2}^{r} z_j\right).$$

On the other hand, we have

$$Zw_1 = z_1 - \sum_{j=2}^{r} \frac{1}{r-1} z_j.$$

Combining these latter two facts gives us

$$Zw_1 = \left(1 + \frac{1}{r-1}\right) z_1 - \frac{1}{r-1} e_n.$$

Similarly, we obtain for $i = 1, \ldots, r, i \neq k$,

$$Zw_i = z_i - \sum_{j \neq i} \frac{1}{r-1} z_j,$$

and, therefore,

$$Zw_i = \left(1 + \frac{1}{r-1}\right) z_i - \frac{1}{r-1} e_n.$$

Hence,

$$ZW = [\alpha z_1, \ldots, \alpha z_{k-1}, \alpha z_{k+1}, \ldots, \alpha z_r] - \frac{1}{r-1} e_n e_{r-1}^T, \quad \alpha := 1 + \frac{1}{r-1}. \tag{3.8}$$

Suppose now that

$$\bar{Z} := [\alpha z_1, \ldots, \alpha z_{k-1}, \alpha z_{k+1}, \ldots, \alpha z_r] = \alpha \widetilde{Z}.$$

Then, with Eq. (3.4) and since e_n is in the null space of A, we get

$$W^T Z^T AZW = \bar{Z}^T A\bar{Z}.$$

The columns of W form a basis of the orthogonal complement of $\mathcal{N}(E)$. Using Theorem 3.8, we obtain that $\bar{Z}^T A\bar{Z}$ is nonsingular. From Eqs. (3.4) and (3.8), we obtain $AZW = A\bar{Z}$. Thus,

$$AZW(W^T Z^T AZW)^{-1}W^T Z^T A = A\bar{Z}(\bar{Z}^T A\bar{Z})^{-1}\bar{Z}^T A.$$

Since $\bar{Z} = \alpha\widetilde{Z}$ holds, we have

$$A\bar{Z}(\bar{Z}^T A\bar{Z})^{-1}\bar{Z}^T A = A\widetilde{Z}(\widetilde{Z}^T A\widetilde{Z})^{-1}\widetilde{Z}^T A.$$

Using Theorem 3.8 we get

$$AZ(Z^T AZ)^+ Z^T A = A\widetilde{Z}(\widetilde{Z}^T A\widetilde{Z})^{-1}\widetilde{Z}^T A.$$

Consequently,

$$P_+ A = \widetilde{P}A. \qquad \square$$

So, for this special situation one only needs to remove a column of Z to get a nonsingular coarse grid matrix. As a special case we get the following corollary.

Corollary 3.10. *Let A be SPSD and $Z \in \mathbb{R}^{n\times r}$, $r \geq 2$ be given such that*

$$Ae_n = 0; \tag{3.9}$$

$$Ze_r = e_n; \tag{3.10}$$

$$\operatorname{rank} A = n - 1; \tag{3.11}$$

$$\operatorname{rank} E = r - 1. \tag{3.12}$$

Suppose that

$$\widetilde{Z} = [z_1, \ldots, z_{r-1}], \quad Z = [\widetilde{Z},\ z_r].$$

Moreover, we define

$$\widetilde{P} := I - A\widetilde{Q}, \quad \widetilde{Q} := \widetilde{Z}\widetilde{E}^{-1}\widetilde{Z}^T, \quad \widetilde{E} := \widetilde{Z}^T A\widetilde{Z}.$$

Then, $\widetilde{E}$ is nonsingular and the following equalities hold:

$$AQ_+ A = A\widetilde{Q}A, \quad P_+ A = \widetilde{P}A,$$

where Q_+ and P_+ are defined as in Eq. (1.2).

The statement of Corollary 3.10 is first stated in [22]. However, the proof given in [22] is not correct. There, the result used the fact that the projection matrix P_+ is independent of the choice of the basis of the column space of Z. This certainly holds for a SPD matrix A, but it is generally not true for a singular coefficient matrix, A. Here we have used a completely different approach that is based on our more general theorems proved in the previous subsection.

3.5. Spectral properties

We consider the spectrum of P_+A, denoted by $\sigma(P_+A)$. The next theorem gives some more information about the spectrum of P_+A.

Theorem 3.11. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD and satisfy $\dim \mathcal{N}(A) = s$. Moreover, suppose that $Z \in \mathbb{R}^{n\times r}$ is of full rank and given such that $\operatorname{rank}(Z^TAZ) = t$. Then,*

$$\sigma(P_+A) = \{0, \dots 0, \lambda_{s+t+1}, \dots \lambda_n\},$$

where $s + t \geq r$ and the eigenvalues λ_i of P_+A, $i = s + t + 1, \dots, n$, are positive.

Proof. Note first that

$$P_+AZE^+ = P_aAZ_a = 0,$$

where P_a and Z_a are defined as in the proof of Theorem 3.6. Moreover, Z_a has full rank, i.e., $\operatorname{rank} Z_a = t$ so that we have t linear independent eigenvectors corresponding to the eigenvalue zero. With Proposition 3.5, i.e. $\mathcal{N}(A) \cap \mathcal{R}(Z_a) = \{0\}$, we obtain

$$\sigma(P_+A) = \{0, \dots 0, \lambda_{s+t+1}, \dots \lambda_n\}.$$

Next, we will show that $s + t \geq r$. We define a matrix $R \in \mathbb{R}^{n\times(n-r)}$ such that $X = [Z, R]$ is a nonsingular matrix. Then, this gives us

$$X^TAX = \begin{bmatrix} Z^TAZ & Z^TAR \\ R^TAZ & R^TAR \end{bmatrix}.$$

Because E is SPSD and $\operatorname{rank}(E) = t$, we have $\dim \mathcal{N}(E) = r - t$. Therefore, using Lemma 2.7,

$$\dim \mathcal{N}(X^TAX) \geq r - t.$$

Then, Lemma 2.6 yields

$$\dim \mathcal{N}(A) = s \geq r - t.$$

Thus,

$$\sigma(P_+A) = \{0, \dots 0, \lambda_{s+t+1}, \dots \lambda_n\},$$

with $\lambda_i \geq 0$. □

Note that if there is no information given about the dimension of the null space of A, we still have

$$\sigma(P_+A) = \{0, \dots 0, \lambda_{r+1}, \dots \lambda_n\}.$$

4. Projection and coarse-grid correction methods

As mentioned earlier in the introduction, an efficient preconditioner consists of a two-level or multi-level structure, see also [23] and the references therein. An example of such a two-level deflation preconditioner is used in the deflation method and is denoted by

$$\mathcal{P}_{\text{DEF1}} = M^{-1}P.$$

Following the derivation of the deflation method in [7,19], an alternative two-level preconditioner is

$$\mathcal{P}_{\text{DEF2}} = P^T M^{-1}.$$

In general, each two-level preconditioner combines a traditional preconditioner with a coarse-grid or subspace correction. This combination can be done in several ways. An additive combination leads to the additive coarse grid correction (AD) preconditioner, $\mathcal{P}_{\text{AD}}$, given by

$$\mathcal{P}_{\text{AD}} = M^{-1} + Q. \tag{4.1}$$

A multiplicative combination leads to the so-called abstract balancing Neumann–Neumann (BNN) preconditioner,

$$\mathcal{P}_{\text{BNN}} = P^T M^{-1} P + Q. \tag{4.2}$$

Moreover, we can also derive

$$\begin{cases} \mathcal{P}_{\text{A-DEF1}} &= M^{-1}P + Q; \\ \mathcal{P}_{\text{A-DEF2}} &= P^T M^{-1} + Q; \\ \mathcal{P}_{\text{R-BNN1}} &= P^T M^{-1} P; \\ \mathcal{P}_{\text{R-BNN2}} &= P^T M^{-1}, \end{cases}$$

Table 1
List of methods which will be compared. If possible, references to the methods, for SPD matrices, and their implementations are given in the last column.

Name	Method	Two-level preconditioner	References
PREC	Traditional PCG	M^{-1}	[4,12]
AD	Additive coarse-grid correction	$M^{-1} + Q_+$	[2,24,20]
DEF1	Deflation variant 1	$M^{-1}P_+$	[26]
DEF2	Deflation variant 2	$P_+^T M^{-1}$	[7,17,19]
A-DEF1	Adapted deflation variant 1	$M^{-1}P_+ + Q_+$	[20]
A-DEF2	Adapted deflation variant 2	$P_+^T M^{-1} + Q_+$	[20]
BNN	Abstract balancing	$P_+^T M^{-1} P_+ + Q_+$	[9]
R-BNN1	Reduced balancing variant 1	$P_+^T M^{-1} P_+$	–
R-BNN2	Reduced balancing variant 2	$P_+^T M^{-1}$	[9,24]

which are the so-called adapted versions of the deflation method and the reduced variants of the BNN method, respectively. These two-level preconditioners appear frequently in the fields of deflation, multigrid and domain decomposition, where their components of the preconditioners usually have their own interpretation and optimized choices. In this paper, we assume that these components are abstract expressions, so that the methods can be compared fairly.

Using the abstract forms of the two-level preconditioners, they have been compared theoretically and numerically in [23], where it has been assumed that A is a nonsingular matrix. Here, we extend this comparison to singular SPSD matrices. Therefore, we introduce the two-level preconditioners that have the same structure as the ones given above, but we now use P_+ and Q_+ instead of P and Q, respectively. These methods are also presented in Table 1, which is an generalization of [23, Table 2.2]. Some specific methods of these type are already analysed for singular matrices, see [8].

The results in Section 3.3 can be used to show that most of the theory for SPD matrices as presented in [23] is also valid for SPSD matrices. One can use the reduced deflation-subspace matrix, Z_a, to find a reduced nonsingular matrix Q_a, so that the theory in [14,15,23] can be followed by observing that the nonsingularity of A is not used in the proofs of many results. With the adaptations, the resulting proofs are very close to them based on the SPD case. Therefore, we do not provide all proofs explicitly, but we state only the results below.

We start with a comparison of the deflation and the additive coarse-grid correction preconditioner.

Theorem 4.1. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD with $\dim \mathcal{N}(A) = s$. Let $M \in \mathbb{R}^{n\times n}$ be SPD. Let $Z \in \mathbb{R}^{n\times r}$ with $\operatorname{rank} E = t$ be given. Suppose that P_+ and Q_+ are defined as in (1.2). Then, the deflation preconditioner defined in (1.2) and the additive coarse-grid correction preconditioner satisfy*

$$\lambda_n(M^{-1}P_+A) \leq \lambda_n((M^{-1} + Q_+)A); \tag{4.3}$$

$$\lambda_{s+t+1}(M^{-1}P_+A) \geq \lambda_{s+1}((M^{-1} + Q_+)A). \tag{4.4}$$

Proof. The proof follows from Lemma 2.4 and the proof of [14, Thm. 2.12]. □

Thus, as in the SPD case, the deflation method provides the same or a better effective condition number than the additive coarse grid correction, so a faster convergence rate of the deflation method is expected.

Subsequently, we show that some of the projection methods lead to exactly the same spectra, see the next theorem.

Theorem 4.2. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD. Suppose that P_+ and Q_+ are defined as in (1.2). Then, the following two statements hold:*

- $\sigma\left(M^{-1}P_+A\right) = \sigma\left(P_+^TM^{-1}A\right) = \sigma\left(P_+^TM^{-1}P_+A\right)$;
- $\sigma\left((P_+^TM^{-1}P_+ + Q_+)A\right) = \sigma\left((M^{-1}P_+ + Q_+)A\right) = \sigma\left((P_+^TM^{-1} + Q_+)A\right)$.

Proof. Note first that $\sigma(CD) = \sigma(DC)$, $\sigma(C + I) = \sigma(C) + \sigma(I)$ and $\sigma(C) = \sigma(C^T)$ hold for arbitrary matrices $C, D \in \mathbb{R}^{n\times n}$. Using these facts and Lemma 3.1, we obtain immediately

$$\sigma\left(M^{-1}P_+A\right) = \sigma\left(AM^{-1}P_+\right) = \sigma\left(P_+^TM^{-1}A\right),$$

and

$$\begin{aligned}\sigma\left(M^{-1}P_+A\right) &= \sigma\left(M^{-1}P_+^2A\right)\\ &= \sigma\left(M^{-1}P_+AP_+^T\right)\\ &= \sigma\left(P_+^TM^{-1}P_+A\right),\end{aligned}$$

which proves the first statement. Moreover, we have

$$\begin{aligned}\sigma\left(P_+^TM^{-1}P_+A + Q_+A\right) &= \sigma\left(P_+^TM^{-1}P_+A - P_+^T + I\right)\\ &= \sigma\left((M^{-1}P_+A - I)P_+^T\right) + \sigma(I)\\ &= \sigma\left(M^{-1}P_+^2A - P_+^T\right) + \sigma(I)\\ &= \sigma\left(M^{-1}P_+A + Q_+A\right),\end{aligned}$$

and, likewise,

$$\begin{aligned}\sigma\left(P_+^TM^{-1}A + Q_+A\right) &= \sigma\left(P_+^TM^{-1}A - P_+^T\right) + \sigma(I)\\ &= \sigma\left(AM^{-1}P_+ - P_+\right) + \sigma(I)\\ &= \sigma\left(P_+AM^{-1}P_+ - P_+\right) + \sigma(I)\end{aligned}$$

$$= \sigma\left(P_+^T M^{-1} A P_+^T - P_+^T\right) + \sigma(I)$$
$$= \sigma\left(P_+^T M^{-1} P_+ A + Q_+ A\right),$$

which completes the proof of the second statement. □

From Theorem 4.2, we have the result that there are two groups of methods in which each two-level preconditioner of the same group leads to the same spectra. The next theorem gives a connection between these two spectra.

Theorem 4.3. *Let $A \in \mathbb{R}^{n\times n}$ be SPSD with $\dim \mathcal{N}(A) = s$. Let $M \in \mathbb{R}^{n\times n}$ be SPD. Let $Z \in \mathbb{R}^{n\times r}$ with $\operatorname{rank} E = t$ be given. Suppose that the spectrum of the two-level preconditioned matrix of DEF1, DEF2, R-BNN1 or R-BNN2 is given by*

$$\sigma = \{0, \ldots, 0, \mu_{s+t+1}, \ldots, \mu_n\}.$$

Then, the spectrum of the two-level preconditioned matrix of A-DEF1, A-DEF2 or BNN is

$$\sigma(P_{B_+} A) = \{0, \ldots, 0, 1, \ldots, 1, \mu_{s+t+1}, \ldots, \mu_n\},$$

with s zeros. Moreover, the converse statement is also true.

Proof. The proof is the same as the proof of [15, Theorem 2.8]. □

As mentioned in [23] for SPD matrices, some of the two-level preconditioners provide the same approximations of CG if a specific starting vector is used. This can be easily generalized to SPSD matrices, see the next theorem.

Theorem 4.4. *DEF2, A-DEF2, R-BNN1 or R-BNN2 based on an SPSD matrix A and the starting vector $Q_+ b + P_+^T \bar{x}$ for an arbitrary vector $\bar{x}$ produces the same iterates in exact arithmetic as BNN based on the starting vector $\bar{x}$.*

Proof. The proof is similar to the proof of [23, Corollary 3.2]. □

5. Conclusions

We have shown that the deflation and other projection methods can deal with general singular coefficient matrices. The projection that is usually based on a singular Galerkin matrix can always be written as a projection that uses a nonsingular Galerkin matrix. This means that many theoretical results for SPD matrices can be easily generalized for SPSD matrices. We have seen that the singularity of the coefficient matrix does not influence the convergence behavior of and the relations between the projection methods in exact arithmetic.

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