PROJECTED KRYLOV METHODS BETWEEN TWO SUBSPACES

Radek Kučera, Tomáš Kozubek, Alexandros Markopoulos
Jaroslav Haslinger, Lukáš Mocek

VŠB-TU Ostrava
17. listopadu 15, 708 33 Ostrava-Poruba
E-mail: radek.kucera@vsb.cz

Abstract: The contribution deals with the solution of large non-symmetric two-by-two block linear systems with singular (1,1)-blocks. The algorithm consists of two levels. The outer level combines the Schur complement reduction with the orthogonal projectors that leads to the linear equation between two different subspaces. This equation is solved by a Krylov-type method. The efficiency is illustrated by examples arising from the combination of the fictitious domain and FETI method.

1 Introduction

We consider two-by-two block linear systems

$$\begin{pmatrix} A & B_1^\top \\ B_2 & -C \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$, $C \in \mathbb{R}^{m\times m}$, $B_1, B_2 \in \mathbb{R}^{m\times n}$, $f, u \in \mathbb{R}^n$, $g, \lambda \in \mathbb{R}^m$, and $m \ll n$. Systems of this type arise in a variety of scientific and engineering applications [1]. The

This work was supported by the grant GA CR P201/12/0671 (RK,JH), by the project SPOMECH, reg. no. CZ.1.07/2.3.00/20.0070 (TK), and by the project Opportunity for young researchers, reg. no. CZ.1.07/2.3.00/30.0016 (AM) within Operational Programme Education for Competitiveness funded by Structural Funds of the European Union and state budget of the Czech Republic.

algorithm analyzed in this paper extends the algebraic background of the FETI (Finite Element Tearing and Interconnecting) domain decomposition methods [3, 7], in which A is symmetric, positive semidefinite, $B_1 = B_2$, and $C = 0$. Here, we consider the general case with the only one assumption that the block matrix in (1.1) is non-singular while A is singular.

The extension of the FETI algorithm for solving (1.1) with $C = 0$ called the PSCM (Projected Schur Complement Method) was proposed in [5]. The general algorithmical scheme combines the Schur complement reduction with the null-space method performed by orthogonal projectors. It results in the linear equation given by a singular matrix that is an invertible operator between two different subspaces $\mathbb{V}_1$ and $\mathbb{V}_2$ in $\mathbb{R}^m$. Since it is not efficient to assembly the Schur complement for large-scale problems, the only operation allowed with the operator matrix is the matrix-vector multiplication. To this end one can use Krylov-type methods. In [5], the authors proposed the ProjBiCGSTAB with an appropriate combination of orthogonal projectors on $\mathbb{V}_1$ and $\mathbb{V}_2$. Here, we prove the condition for the angle between $\mathbb{V}_2$ and $\mathbb{V}_1^{\perp}$ guaranting the convergence. Our analysis open the door for deriving other projected Krylov methods between subspaces. As an example, we use the projected GMRES in numerical experiments. The efficiency is illustrated by examples arising from the combination of the fictitious domain and FETI method.

2 Deriving of projected Krylov methods

The PSCM algorithm requires to compute actions of an arbitrary generalized inverse X to A and of the matrices R_A, $R_{A^\top}$ whose columns span the null-spaces of A and $A^\top$, respectively [6]. We will assume that $G_1 = -R_A^\top B_2^\top$, $G_2 = -R_{A^\top}^\top B_1^\top$, $d = B_2 X f - g$, and $e = -R_{A^\top}^\top f$ are assembled while $F = B_2 X B_1^\top + C$ is to our disposal by the multiplying procedure. The last ingredients are two orthogonal projectors onto the null-spaces $\mathcal{N}(G_i)$ of G_i denoted by $P_i = I - G_i^\top (G_i G_i^\top)^{-1} G_i$, $i = 1, 2$. The key step of the PSCM algorithm consists in solving of the operator equation

$$P_1 F x = q \tag{2.1}$$

with $q = P_1(d - F G_2^\top (G_2 G_2^\top)^{-1} e)$, where x is the projection of λ onto $\mathcal{N}(G_2)$. Although $P_1 F$ is the singular matrix in $\mathbb{R}^m$, the solvability of (2.1) is guaranteed, as $P_1 F$ is the invertible operator between $\mathcal{N}(G_2)$ and $\mathcal{N}(G_1)$ [5, 6].

Let $\mathbb{V}_1, \mathbb{V}_2 \subset \mathbb{R}^m$ be two different subspaces of the same dimension $m - l$, $1 \le l < m$. We replace (2.1) by the following abstract problem: find $x \in \mathbb{V}_2$ such that

$$Mx = q, \tag{2.2}$$

where $q \in \mathbb{V}_1$ and $M \in \mathbb{R}^{m \times m}$ represents the invertible operator between $\mathbb{V}_1$ and $\mathbb{V}_2$. Let $Z_1, Z_2 \in \mathbb{R}^{m \times (m-l)}$ be matrices whose columns span $\mathbb{V}_1$, $\mathbb{V}_2$, respectively. Let $\bar{x}, \bar{q} \in \mathbb{R}^{m-l}$ be such that $q = Z_1 (Z_1^\top Z_1)^{-1} \bar{q}$, $x = Z_2 \bar{x}$. Substituting these vectors into (2.2) and multiplying by $Z_1^\top$, we find that (2.2) reduces to the system of linear equations:

$$N\bar{x} = \bar{q}, \tag{2.3}$$

where $N = Z_1^\top M Z_2 \in \mathbb{R}^{(m-l)\times(m-l)}$.

Lemma 2.1 *The matrix N in (2.3) is non-singular.*

Proof. Let $Z_1^\top M Z_2 y = 0$ be the homogeneous system. Denoting $y_1 = M Z_2 y$, we obtain $Z_1^\top y_1 = 0$. As $y_1 \in \mathbb{V}_1$ is orthogonal to all basis vectors of $\mathbb{V}_1$, we get $y_1 = 0$. In $M Z_2 y = 0$, we set $y_2 = Z_2 y$. Then, $M y_2 = 0$ implies $y_2 = 0$ due to the invertibility of M. Finally, $Z_2 y = 0$ yields $y = 0$, as Z_2 has full column-rank. Hence, the solution to the homogeneous system is trivial. $\square$

A (standard) Krylov method applied to (2.3) generates approximations to the solution $\bar{x}$ of (2.3) in $\mathbb{R}^{m-l}$. The projected Krylov method generates approximations directly to the solution x of (2.2) in $\mathbb{V}_2$. The crucial point in deriving projected methods consists in showing how to transform the matrix-vector multiplication from $\mathbb{R}^{m-l}$ to $\mathbb{V}_2$. The idea is based on the following equivalences:

$$\bar{y} = Z_1^\top M Z_2 \bar{x} \quad \Longleftrightarrow \quad Z_2 \bar{y} = Z_2 Z_1^\top M Z_2 \bar{x} \quad \Longleftrightarrow \quad y = Z_2 Z_1^\top M x. \tag{2.4}$$

Let $M_P \in \mathbb{R}^{m\times m}$ be another invertible operator between V_2 and $\mathbb{V}_1$. We can consider Z_2 orthogonal and introduce $Z_1 = M_P Z_2$. Taking into account $P_2 = Z_2 Z_2^\top$, we get

$$y = P_2 M_P^\top M x. \tag{2.5}$$

We discuss two variants of M_P: *(i)* $M_P = M$ and *(ii)* $M_P = P_1$.

The variant *(i)* leads to N non-singular for any choice of the input data and enables us to use the CGM. On the other hand, two expensive matrix-vector multiplications by M and $M^\top$ are needed in (2.5). Moreover, the condition number $\kappa(N)$ is usually too high so that the convergence rate of the CGM may be slow.

For the variant *(ii)*, the invertibility of M_P is guaranteed by the following result.

Theorem 2.1 *Let P_1 be the orthogonal projector onto $\mathbb{V}_1$. The restriction $P_1 : \mathbb{V}_2 \mapsto \mathbb{V}_1$ is invertible iff*

$$\mathbb{V}_2 \cap \mathbb{V}_1^\perp = \{0\}, \tag{2.6}$$

where $\mathbb{V}_1^\perp$ is the orthogonal complement to $\mathbb{V}_1$ in $\mathbb{R}^m$.

Proof. First we prove the implication "$\Leftarrow$". Any $x \in \mathbb{V}_2$ can be split into two orthogonal components: $x = x_{\mathbb{V}_1^\perp} + x_{\mathbb{V}_1}$, where $x_{\mathbb{V}_1^\perp} \in \mathbb{V}_1^\perp$ and $x_{\mathbb{V}_1} \in \mathbb{V}_1$. If $x \neq 0$, then (2.6) yields $x_{\mathbb{V}_1} \neq 0$ and $P_1 x = x_{\mathbb{V}_1}$. Therefore, the only solution of the homogeneous equation $P_1 x = 0$ on $\mathbb{V}_2$ is trivial. The invertibility of P_1 on $\mathbb{V}_2$ is proved. To prove the opposite implication "$\Rightarrow$", we assume that there is $x \in \mathbb{V}_2 \cap \mathbb{V}_1^\perp$, $x \neq 0$. Then, x is the non-zero solution of the homogeneous equation $P_1 x = 0$ on $\mathbb{V}_2$. This contradicts to the invertibility of P_1 on $\mathbb{V}_2$. $\square$

The condition (2.6) is equivalent to the fact that the angle θ between $\mathbb{V}_2$ and $\mathbb{V}_1^\perp$ is non-zero. It is implicitly required by ProjBiCGSTAB proposed in [5]. It is possible to prove that N is close to a singular matrix when θ is small. In such situations, the convergence rate of the projected Krylov methods may be slow. However, if θ is sufficiently large, then the variant *(ii)* may avoid disadvantages of *(i)*.

3 Numerical experiments

To test our algorithms, we shall solve linear systems (1.1) arising from the combination of the smooth FD and FETI method applied to finite element approximations of linear elasticity problems [5, 4, 8].

We compare the efficiency of the PSCM implemented with different projected Krylov methods used for solving (2.1). By ProjGMRES(P_1F) and ProjGMRES(P_1) we denote the projected GMRES variants with $M_P = M$ and $M_P = P_1$, respectively. Note that the former leads to the equation with the symmetric, positive definite operator so that the projected CGM may be also used in this case. We refer to this method as ProjCGM(P_1F). The projected BiCGSTAB [5] is denoted here by ProjBiCGSTAB(P_1). Actions of generalized inverses of A to vectors are computed by combining the Cholesky factorization with the singular value decomposition [2]. The choice of the generalized inverse has no influnce on convergence of the projected methods [7, 6]. All computations were performed by using 32 cores with 2GB memory per core of the HP Blade system, model BLc7000.

Figure 3.1 and 3.2 show convergence rate of the relative residual norm which is typical for small and large problems, respectively. Table 3.1 reports the number of iterations (**iter**) and the computational time in seconds (CPU_time). One can observe that ProjGMRES(P_1) is the most efficient method, if a high accuracy of the computed solution is required. The progress is more expressive in CPU_time, since the only one action of the generalized inverse of A per iteration is needed.

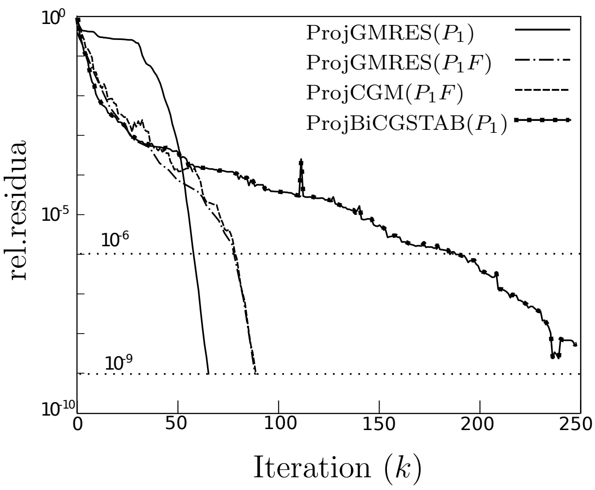

Figure 3.1: $n = 3528$, $m = 186$.

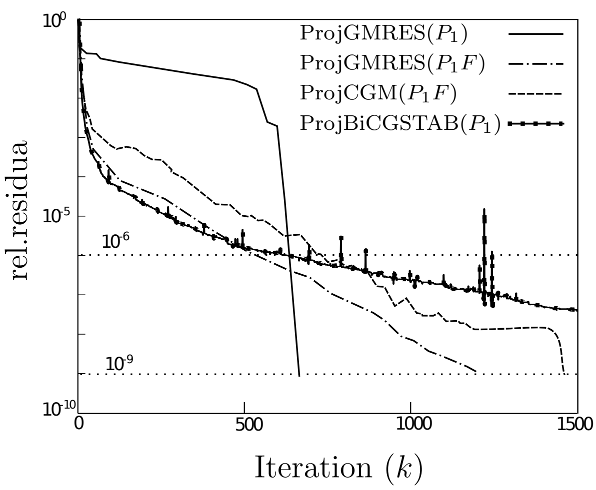

Figure 3.2: $n = 520200$, $m = 18372$.

References

[1] M. Benzi, G.H. Golub, J. Liesen, Numerical solution of saddle point systems, Acta Numerica 14 (2005) 1–137.

	25	100	225
number of the subboxes (s)	25	100	225
number of the primal unknowns (n)	130050	520200	1170450
number of the dual unknowns (m)	4148	18372	42692
nullity of A (l)	75	300	675
$\varepsilon = 10^{-6}$			
ProjGMRES(P_1)	**322**/34.68	**633**/289.36	**1001**/2474.12
ProjGMRES(P_1F)	**289**/48.52	**543**/396.74	**743**/2164.29
ProjCGM(P_1F)	**378**/63.34	**732**/588.48	**1046**/4339.76
ProjBiCGSTAB(P_1)	**538**/163.55	**628**/793.28	**672**/1849.82
$\varepsilon = 10^{-9}$			
ProjGMRES(P_1)	**342**/35.86	**665**/327.45	**1040**/2817.11
ProjGMRES(P_1F)	**592**/122.63	**1210**/1100.40	**1678**/7462.21
ProjCGM(P_1F)	**686**/126.80	**1462**/1242.95	**2198**/9666.65
ProjBiCGSTAB(P_1)	>1500	>1500	>1500

Table 3.1: Complexity of computations: **iter**/CPU_time for two terminating tolerances ε (if >1500, the default maximum of iterations is achieved).

[2] T. Brzobohatý, Z. Dostál, T. Kozubek, A. Markopoulos, P. Kovář, Cholesky decomposition with fixing nodes to stable evaluation of a generalized inverse of the stiffness matrix of a floating structure, International Journal for Numerical Methods in Engineering 88 (2011) 1384–1405.

[3] C. Farhat, J. Mandel, F.X. Roux, Optimal convergence properties of the FETI domain decomposition method, Comput. Methods Appl. Mech. Engrg. 115 (1994) 367–388.

[4] J. Haslinger, T. Kozubek, R. Kučera, Fictitious domain formulation of unilateral problems: analysis and algorithms, Computing 84 (2009) 69–96.

[5] J. Haslinger, T. Kozubek, R. Kučera, G. Peichl, Projected Schur complement method for solving non-symmetric saddle-point systems arising from fictitious domain approach, Numerical Linear Algebra with Applications 14 (2007) 713–739.

[6] R. Kučera, T. Kozubek, A. Markopoulos, On large-scale generalized inverses in solving two-by-two block linear systems, Linear Algebra and Its Applications 438 (2013) 3011–3029.

[7] R. Kučera, T. Kozubek, A. Markopoulos, J. Machalová, On the Moore-Penrose inverse in solving saddle-point systems with singular diagonal blocks, Numerical Linear Algebra with Applications 19 (2012) 677–699.

[8] L. Mocek, Numerical solution of partial differential equations using a fictitious domain method, PhD Thesis, VSB-TU Ostrava, 2012. At: *http://www.fei.vsb.cz/miranda2/export/sites-root/fei/k470/cs/theses/mocek_phd.pdf*