AN ITERATIVE PROCEDURE FOR COMPUTING THE NULL BASIS

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Abstract. We are interested in the computation of a basis for the null space (the so-called *null basis*) of a real square matrix A with $\text{ind}(A) = 1$, by means of an iterative procedure. No a priori knowledge is assumed on the dimension of the null space, therefore the method starts with a guess basis size and then adjusts its value as the iteration proceeds. The kernel is a short-term recurrence algorithm based on the Krylov subspace that allows to determine independent vectors of the null basis. Theoretical justification is provided, and results from first experimental tests are reported.

1. Introduction. We are interested in the computation of a basis for the null space (the so-called *null basis*) of a real square matrix A of size N. Denoting by $r \geq 0$ the dimension of the null space of A, we look for a full rank matrix $X \in \mathbb{R}^{N\times r}$ such that

$$AX = 0. \tag{1.1}$$

We do not assume any a priori knowledge on the dimension of the null space, therefore nonsingular matrices are also included. The null basis finds applications in many practical problems, such as constrained optimization; See for instance [1, 6] and references therein. For A of moderate size, direct methods can be successfully applied to (1.1) [3, 1, 6]. In particular, common approaches consist of either computing the right singular vectors of A corresponding to its zero singular values or determining a QR decomposition of A [4]. If N is large, then iterative methods that determine an approximation $\tilde{X}$ to X are more suitable, since they only require matrix-matrix products with A. The goodness of the approximation can be monitored by, for instance, requiring that the residual $A\tilde{X}$ be small in some sense.

Let $\text{ind}(A)$ be the size of the largest Jordan block of A associated with the zero eigenvalue. For $\text{ind}(A) = 1$, it was shown in [5] that Krylov subspace methods can be used to solve (1.1) for $r = 1$ for any non-zero starting approximation $\tilde{X}_0$. It can be proved that an analogous result holds for $r \geq 1$. The general case with $\text{ind}(A) \geq 1$ causes some difficulties when using Krylov subspace methods [5]. In this paper we propose an iterative procedure that determines $\tilde{X}$ by computing $k \in \mathbb{N}$ vectors of the basis at the time with a block Krylov subspace method, under the constraint $\text{ind}(A) = 1$. We will also explore some specific properties of iterative methods that reveal themselves when solving (1.1). Moreover, we show how subspace perturbation analysis can be naturally applied to this problem in the Krylov subspace setting. We remark that the precision with which a basis of the null space of a matrix is computed is a practical constraint in its application; see the discussion in [23] and some applications in [22, 8].

The paper is organized as follows. Section 2 is devoted to the perturbation analysis associated to the computed basis, with specific interest in the determination of the dimension of the null space of A. In Section 3 Krylov subspace methods on blocks of vectors are discussed, and the equivalence of different approaches is shown. In Section 3.1 a Krylov subspace method for solving $AY = B$ with $Y \in \mathbb{R}^{N\times k}$ is reviewed. The iterative algorithm for computing $\tilde{X}$ is presented in Section 4, and first experiments are reported in Section 5. Finally, open issues are discussed in Section 6.

2. On the approximation of the null space. For any $\varepsilon > 0$, let $\tilde{X} \in \mathbb{R}^{N\times k}$, $\tilde{X}^T\tilde{X} = I$, be such that $\|A\tilde{X}\|_2 = \varepsilon$, where I denotes the identity matrix of prescribed size. For the moment we assume that $k = r := \dim(\mathcal{N}(A))$. Function $\|\cdot\|_2$ denotes the spectral norm

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for matrices and vectors, that is, for $\tilde{X} \in \mathbb{R}^{m\times n}$, $||\tilde{X}||_2 = \max_{y\in\mathbb{R}^n, y\neq 0} ||\tilde{X}y||_2/||y||_2$, and $||y||_2^2 = \sum_{i=1}^N y_i^2$. In the following we shall also employ the Frobenius norm $||\tilde{X}||^2 = \sum_{i=1}^m \sum_{j=1}^n \tilde{x}_{i,j}^2$. Matrix $\tilde{X}$ can be viewed as the exact solution of the perturbed problem $(A+E)\tilde{X} = 0$ for some $E \in \mathbb{R}^{N\times N}$. In [25], Sun carried out a backward perturbation analysis for invariant subspaces of A in order to find the matrix E with smallest norm that exactly solves the associated eigenvalue problem. The theory developed inthere readily applies to problem (1.1), where X corresponds to a basis for the invariant subspace of the zero eigenvalue. Moreover, in [25] optimal backward perturbations are also determined for singular subspaces. Such approach yields an equivalent solution to the problem under the hypothesis that ind$(A) = 1$, which will be assumed throughout the paper. We are particularly interested in the singular subspaces technique because it determines a parametrization for E and the optimal perturbation for both $\mathcal{N}(A)$ and $\mathcal{N}(A^T)$. This will be used in later sections in order to evaluate the goodness of the approximation from a backward perturbation analysis point of view. The result in [25] of interest is recalled below, with simple variants which are due to the presence of the zero singular triples.

THEOREM 2.1 ([25]). [1] *Let $A \in \mathbb{R}^{N\times N}$, r =dim$(\mathcal{N}(A))$, and $\tilde{X}, \tilde{Y} \in \mathbb{R}^{N\times r}$, $\tilde{X}^T\tilde{X} = I = \tilde{Y}^T\tilde{Y}$. Define $\mathcal{E} = \{E \in \mathbb{R}^{N\times N} : (A+E)\tilde{X} = 0, (A+E)^T\tilde{Y} = 0\}$ and let $R_E = -A\tilde{X}$, $Q_E = -A^T\tilde{Y}$ be the residuals of A with respect to $\tilde{X}$ and $\tilde{Y}$. Then any $E \in \mathcal{E}$ has the form $E = -\tilde{Y}(\tilde{Y}^T A\tilde{X})X^T + R_E\tilde{X}^T + \tilde{Y}Q_E^T + (I - \tilde{Y}\tilde{Y}^T)Z(I - \tilde{X}\tilde{X}^T)$ with $Z \in \mathbb{R}^{N\times N}$. Moreover,*

$$E_{(0)} := \begin{cases} R_E\tilde{X}^T & \textit{if } ||R_E\tilde{X}^T||_2 \geq ||\tilde{Y}Q_E^T||_2 \\ \tilde{Y}Q_E^T & \textit{otherwise} \end{cases}, \qquad ||E_{(0)}||_2 = \min_{E\in\mathcal{E}} ||E||_2.$$

We would like to remark that results in accordance to the ones stated above were proved in [12]. However, Theorem 2.1 requires less strict assumptions than in [12] in the case of zero singular values. It is worth to observe that in our setting $||E||_2$ indicates how much degenerate A is, in some respect. The connection between the result in [12] and that in [25] follows from the computation of $E_{(0)}$ for which $\min_{E\in\mathcal{E}} ||E||_2 = \max\{||R_E||_2, ||Q_E||_2\}$.

The fact that $\tilde{X}$ is full rank yields that dim$(\mathcal{N}(A+E)) \geq r$. We next examine a sufficient condition for dim$(\mathcal{N}(A+E)) = r$ to be satisfied. Let $\mathcal{P}$ be the orthogonal projection onto $\mathcal{N}(A)$ and $\mathcal{P}_\perp$ be the projector onto its complementary space. Given a perturbed matrix $\tilde{A} = A + E$, we denote by $\tilde{\mathcal{P}}$, $\tilde{\mathcal{P}}_\perp$ the corresponding projectors for $\tilde{A}$. If X is an orthonormal $N \times r$ matrix such that $AX = 0$, then $\mathcal{P}$ is uniquely determined by $\mathcal{P} = XX^T$. For computational purposes, it is of interest that $\tilde{\mathcal{P}}$ does not have components in $\mathcal{R}(A)$. The following inequality gives insight in understanding the dependence between $\tilde{\mathcal{P}}$ and $\mathcal{P}$ (cf. [24]). Here and in the rest of the paper, $\sigma_1(A), \sigma_{min}(A)$ will denote the largest and smallest (non-zero) singular values of A, respectively.

PROPOSITION 2.2. *Let $\mathcal{P}, \tilde{\mathcal{P}}$ be the orthogonal projections onto $\mathcal{N}(A)$ and $\mathcal{N}(\tilde{A})$, respectively, with $\tilde{A} = A + E$. Then*

$$||\mathcal{P}_\perp\tilde{\mathcal{P}}||_2 \leq \frac{||E||_2}{\sigma_{min}(A)}. \tag{2.1}$$

Proof. Let $A^\dagger$ denote the pseudo-inverse of A. We have $||\mathcal{P}_\perp\tilde{\mathcal{P}}||_2 = ||(I-\mathcal{P})\tilde{\mathcal{P}}||_2 = ||A^\dagger A\tilde{\mathcal{P}}||_2 = ||A^\dagger E\tilde{\mathcal{P}}||_2 \leq \sigma_{min}^{-1}(A)||E||_2$. □

Relation (2.1) suggests that the orthogonality between $\mathcal{P}_\perp$ and $\tilde{\mathcal{P}}$ is preserved, with the same accuracy of the solution, unless $\sigma_{min}(A)$ is very small. Moreover, ([24, Th.

[1] We thank one of the referees for suggesting the current formulation of the theorem.

I.5.5]) $\|\tilde{\mathcal{P}} - \mathcal{P}\|_2 = \|\mathcal{P}_\perp \tilde{\mathcal{P}}\|_2$ which, in view of (2.1), implies $\|\tilde{\mathcal{P}} - \mathcal{P}\|_2 \le \frac{\|E\|_2}{\sigma_{min}(A)}$. For $\sigma_{min}(A)$ not too small, this ensures that $\|\tilde{\mathcal{P}} - \mathcal{P}\|_2 < 1$, which is equivalent to the fact that $\dim(\mathcal{N}(\tilde{A})) = \dim(\mathcal{N}(A))$ ([24, Th. III.3.1]). This sufficient condition is summarized in the following corollary.

COROLLARY 2.3. *Let $\|E\|_2 = \delta$ and suppose that $\delta < \sigma_{min}(A)$. Then*

$$\mathit{dim}(\mathcal{N}(\tilde{A})) = \mathit{dim}(\mathcal{N}(A)). \tag{2.2}$$

Relation (2.2) together with the results of Theorem 2.1 will be discussed further in the experiments section. Analogous requirements can be proved for $\dim(\mathcal{N}(A^T))$.

3. The Krylov subspace approach. In order to solve (1.1), we would like to use an iterative method based on the block Krylov subspace $\mathbb{K}_m(A, V_0) = \text{span}\{V_0, AV_0, \ldots, A^{m-1}V_0\}$, where $V_0 \in \mathbb{R}^{N\times k}$, $k \in \mathbb{N}$. In this section we will limit ourselves to the case $k = r$, and postpone the discussion for general k to the experiments section.

The block Arnoldi method, based on $\mathbb{K}_m(A, V_0)$, can be used to detect approximation to the invariant subspace corresponding to the zero Jordan block of A; See [20] and references therein. Known convergence properties of the block Arnoldi process would be sufficient to justify the use of block Krylov subspace methods in the eigenvalue setting. Moreover, other approaches such as SVD in the Krylov subspace could be considered for this problem. We would like to show next that for $\text{ind}(A) = 1$, a yet different strategy based on block linear system solvers can be more appropriate from a computational view point.

Given a first guess $X_0 \in \mathbb{R}^{N\times r}$, a typical system solver determines an approximate $X_m = X_0 + Z_m$ to the solution of $AX = B$, where $Z_m \in \mathbb{K}_m(A, R_0)$, with $R_0 = B - AX_0$. In our particular case, $R_0 = -AX_0$, and the system (1.1) becomes $AZ = R_0$, where R_0 obviously belongs to $\mathcal{R}(A)$. The resulting system is consistent and thus can be solved [5]. One then computes X_m by enforcing a minimization or orthogonality condition.

Let $K_m := \mathbb{K}_m(A, X_0)$, $L_m := \mathbb{K}_m(A, -AX_0)$, and denote by $\mathcal{V}_m$ and $\mathcal{W}_m$ the two orthogonal bases of the corresponding Krylov subspaces. It holds that $L_m = -AK_m$ and there exists a triangular matrix $C_m \in \mathbb{R}^{m\times m}$ such that

$$\mathcal{W}_m = -A\mathcal{V}_m C_m. \tag{3.1}$$

Matrix C_m can be determined, for instance, by first computing two upper triangular matrices S_K and S_L satisfying $\mathcal{W}_m = [-AX_0, \ldots, -A^m X_0]S_L$ and $\mathcal{V}_m = [X_0, \ldots, A^{m-1}X_0]S_K$, from which $C_m = S_K^{-1} S_L$ [11].

Let $\mathcal{H}_m, \mathcal{T}_m \in \mathbb{R}^{(m+1)\times m}$ be the block upper Hessenberg matrices determined by the Arnoldi process such that $A\mathcal{V}_m = \mathcal{V}_{m+1}\mathcal{H}_m$ and $A\mathcal{W}_m = \mathcal{W}_{m+1}\mathcal{T}_m$ and let $E_1^T = [I, 0, \ldots, 0]$. Relation (3.1) naturally yields the following correspondence.

PROPOSITION 3.1. *Given $X_0 \in \mathbb{R}^{N\times r}$, let $L_m = \mathit{span}\{-AX_0, -A^2X_0, \ldots, -A^m X_0\}$ and $K_m = \mathit{span}\{X_0, AX_0, \ldots, A^{m-1}X_0\}$. Suppose the problem $\min_{X\in X_0+L_m} \frac{\|AX\|}{\|X\|}$ is solvable. Then*

$$\min_{X\in X_0+L_m} \frac{\|AX\|}{\|X\|} = \min_{X\in K_{m+1}} \frac{\|AX\|}{\|X\|}. \tag{3.2}$$

Proof. Write $\mathcal{V}_{m+1} = [V_0, \ldots, V_m]$ and observe that $X_0 = V_0\chi_0 = \mathcal{V}_{m+1}E_1\chi_0$ and $A\mathcal{W}_m = \mathcal{W}_{m+1}\mathcal{T}_m = -A\mathcal{V}_{m+1}C_{m+1}\mathcal{T}_m$. Hence,

$$\begin{aligned}
\min_{X\in X_0+L_m} \frac{\|AX\|}{\|X\|} &= \min_{Y\in\mathbb{R}^{mr\times r}} \frac{\|A(X_0 + \mathcal{W}_m Y)\|}{\|X_0 + \mathcal{W}_m Y\|} = \min_{Y\in\mathbb{R}^{mr\times r}} \frac{\|A\mathcal{V}_{m+1}(-E_1\chi_0 + C_{m+1}\mathcal{T}_m Y)\|}{\|\mathcal{V}_{m+1}(-E_1\chi_0 + C_{m+1}\mathcal{T}_m Y)\|}. \\
&= \min_{Z\in\mathbb{R}^{(m+1)r\times r}} \frac{\|A\mathcal{V}_{m+1}Z\|}{\|\mathcal{V}_{m+1}Z\|} = \min_{X\in K_{m+1}} \frac{\|AX\|}{\|X\|}.
\end{aligned}$$

The correspondence between Z and Y is possible under the hypothesis that the minimum backward error problem is solvable. This is equivalent to the condition that matrix $\tilde{Z} = ([-E_1\chi_0, C_{m+1}\mathcal{T}_m])^{-1}Z$ have nonsingular first $r \times r$ block. □

It was shown in [13] for $r = 1$ that the problem $\min_{X \in X_0+L_m} \frac{\|AX\|}{\|X\|}$ corresponds to finding the matrix E with smallest norm such that $(A+E)X_m = B$, with $X_m \in X_0 + \mathbb{K}_m(A, R_0)$. In our setting, $B = 0$ and $R_0 = -AX_0$ so that X_m exactly solves the system $(A+E)X_m = 0$. A similar correspondence can be stated for the general case $r \geq 1$. We refer to [13] for the existence and uniqueness analysis of the minimum backward error solution. Equality (3.2) shows that this approach provides the same minimum as an SVD into a Krylov subspace of larger dimension. See for instance [17] as an application of the SVD technique. Let $X_{SVD} = \mathcal{V}_{m+1}Z$ be the SVD solution, and $X_{err} = X_0 + \mathcal{W}_m Y$ be the backward error solution. Then it holds

$$\text{span}\{X_{SVD}\} = \text{span}\{X_{err}\}, \tag{3.3}$$

so that there exists a nonsingular matrix $\alpha \in \mathbb{R}^{r\times r}$ such that $X_{SVD} = X_{err}\alpha$ with X_{SVD} and X_{err} full rank. It is worth to explicitly observe that for $r = 1$, $\alpha = \|X_{err}\|^{-1}$.

As described in [13], the method that implements the left-hand side of (3.2) requires the computation of an orthogonal basis for the Krylov subspace as m increases and thus restart should be applied. Memory demand is also a constraint. Moreover, both approaches in (3.2) seek a full rank matrix satisfying $\min_{X\in X_0+L_m} \frac{\|AX\|}{\|X\|}$, therefore the achieved minimum may be far from zero, if the block size is larger than the null space dimension, that is if $X_0 \in \mathbb{R}^{N\times k}$ with $k > r$. We conclude that, unless $\sigma_1(A)\sigma_{min}(A)^{-1}$ be considerably large, the minimization of the backward error may be too restrictive, although a deeper study of this problem for sensitive matrices still needs to be carried out.

The discussion above motivates the analysis of alternative strategies. The backward error approach is tightly connected to the more commonly used minimum residual method for linear systems. For blocks of vectors the latter can be stated as solving the problem $\min_{X\in X_0+L_m} \|AX\|$ associated to (1.1). The following relation is a generalization to $r > 1$ of the result in [14]; A sketch of the proof is also provided.

PROPOSITION 3.2. *Let $\mathcal{W}_m$ be an orthogonal basis of $L_m = \mathbb{K}_m(A, -AX_0)$ satisfying $A\mathcal{W}_m = \mathcal{W}_{m+1}\mathcal{T}_m$. Let $(\Lambda, U) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{r(m+1)\times r}$ be the smallest block eigenpair of size r of the pencil $(\tilde{\mathcal{T}}_m^T\tilde{\mathcal{T}}_m, [X_0, \mathcal{W}_m]^T[X_0, \mathcal{W}_m])$, with $\tilde{\mathcal{T}}_m = [\mathcal{W}_{m+1}^T(AX_0), \mathcal{T}_m]$ and $u = E_1^T U \in \mathbb{R}^{r\times r}$. Suppose that u is nonsingular, and denote by X_{err} and X_{min} the approximate solutions in L_m of the backward error and minimum residual methods, respectively. Then*

$$X_{min} = X_{err} - \mathcal{W}_m(\mathcal{T}_m^T\mathcal{T}_m)^{-1}\mathcal{W}_m^T X_{err}(u\Lambda u^{-1}).$$

Proof. Using arguments similar to those in [14], it can be shown that matrix Y_{err} in the approximate solution $X_{err} = X_0 + \mathcal{W}_m Y_{err}$ is computed as

$$\begin{bmatrix} I \\ Y_{err} \end{bmatrix} = Uu^{-1} \qquad \text{where} \qquad \tilde{\mathcal{T}}_m^T\tilde{\mathcal{T}}_m U = [X_0, \mathcal{W}_m]^T[X_0, \mathcal{W}_m]U\Lambda.$$

By replacing U in the matrix equation, one obtains

$$\mathcal{T}_m^T\mathcal{W}_m^T(AX_0)u + \mathcal{T}_m^T\mathcal{T}_m Y_{err}u = (\mathcal{W}_m^T X_0 + Y_{err})u\Lambda.$$

Using the fact that matrix Y_{min} of $X_{min} = X_0 + \mathcal{W}_m Y_{min}$ is computed as $\mathcal{T}_m^T\mathcal{T}_m Y_{min} = -\mathcal{T}_m^T\mathcal{W}_m^T(AX_0)$ and that $\mathcal{W}_m^T X_{err} = \mathcal{W}_m^T X_0 + Y_{err}$, it follows

$$\mathcal{T}_m^T\mathcal{T}_m Y_{min}u = \mathcal{T}_m^T\mathcal{T}_m Y_{err}u - \mathcal{W}_m^T X_{err}u\Lambda.$$

Hence, $Y_{min} = Y_{err} - (\mathcal{T}_m^T \mathcal{T}_m)^{-1} \mathcal{W}_m^T X_{err} u \Lambda u^{-1}$, from which the result readily follows. □

The major advantage of the block minimum residual approach is that X_{min} is not necessarily of full rank and therefore the method can converge to the null basis even for larger block size than the dimension of $\mathcal{N}(A)$.

3.1. A short-term recursion. Full minimization of the residual is an optimal requirement but computationally expensive, since it undergoes the same constrains of the minimum backward error method. If one is equivalently satisfied with a quasi-minimization of the residual, then a short-term recurrence can be employed, with low memory load and no restart. Let X_0 be a starting approximate solution and R_0 be the associated residual. Short recurrence iterations are characterized by relations of type

$$A\mathcal{S}_{m-1} = \mathcal{Q}_m \mathcal{T}_m, \quad \mathcal{S}_{m-1} = [S_0, \ldots, S_{m-1}] \in \mathbb{R}^{N \times rm}, \quad \mathcal{Q}_m = [Q_0, \ldots, Q_m] \in \mathbb{R}^{N \times r(m+1)},$$

where, usually, $S_0 = Q_0 \equiv R_0 \xi_0$, and $\mathcal{T}_m \in \mathbb{R}^{(m+1)r \times mr}$ is a block banded matrix. The approximate solution at step m is given by $X_m = X_0 + Z_m$ with $Z_m \in \mathbb{K}_m(A, R_0)$, $Z_m = \mathcal{S}_{m-1} Y_m$, for a certain $Y_m \in \mathbb{R}^{mr \times r}$. The block version of the biconjugate gradients ([16]) satisfies these relations and can be applied on non symmetric matrices. Unfortunately, this method is not always reliable due to loss of orthogonality of the block iterates [21]. In [19] a new version of the block biconjugate gradients algorithm (MBBICG) was presented, which showed better convergence properties than the original implementation. The new method determines approximate solutions for both $AX = B$ and $A^T \tilde{X} = \tilde{B}$ by building the Krylov subspaces $\mathbb{K}_m(A, R_0)$ and $\mathbb{K}_m(A^T, \tilde{R}_0)$, where $\tilde{R}_0$ is the starting residual for the system $A^T \tilde{X} = \tilde{B}$. Four sets of matrices $\{Q_i\}$, $\{\tilde{Q}_i\}$ and $\{S_i\}$, $\{\tilde{S}_i\}$ are iteratively generated so that $\tilde{Q}_i^T Q_i = \Omega_i$, $\tilde{S}_i^T A S_i = \Pi_i$, with Ω_i and Π_i diagonal. At step i, the iterates are updated by means of the relations

$$Q_{i+1}\xi_{i+1} = Q_i - AS_i \Pi_i^{-1} \tilde{\tau}_i^{-T} \Omega_i, \qquad \tilde{Q}_{i+1}\tilde{\xi}_{i+1} = \tilde{Q}_i - A^T \tilde{S}_i \Pi_i^{-T} \tau_i^{-T} \Omega_i^T$$

where $\xi_{i+1}, \tilde{\xi}_{i+1}$ are such that $\tilde{Q}_{i+1}^T Q_{i+1} = \Omega_{i+1}$ is diagonal, and

$$S_{i+1}\tau_{i+1} = Q_{i+1} + (S_i \tau_i) \Omega_i^{-1} \tilde{\xi}_{i+1}^T \Omega_{i+1}, \qquad \tilde{S}_{i+1}\tilde{\tau}_{i+1} = \tilde{Q}_{i+1} + (\tilde{S}_i \tilde{\tau}_i) \Omega_i^{-T} \xi_{i+1}^T \Omega_{i+1}^T$$

with $\tilde{S}_{i+1}^T A S_{i+1} = \Pi_{k+1}$. The approximate solution is computed by imposing a quasi-minimization of the residual norm. Letting $R_0 = Q_0 \xi_0$, the residual $R_i = B - AX_i$ becomes $R_i = \mathcal{Q}_i (E_1 \xi_0 - \mathcal{T}_i Y)$. The block quasi-minimization procedure we use consists of solving the least squares problem

$$\min_{Y \in \mathbb{R}^{ir \times r}} \|\mathcal{W}_i (E_1 \xi_0 - \mathcal{T}_i Y)\|, \tag{3.4}$$

rather than $\|\mathcal{Q}_i (E_1 \xi_0 - \mathcal{T}_i Y)\|$, where $\mathcal{W}_i$ is a weight matrix such that $\mathcal{Q}_i \mathcal{W}_i^{-1}$ has columns of unit norm. Problem (3.4) is solved by doing a QR decomposition of the banded matrix $\mathcal{T}_i = \mathcal{U}_i \mathcal{R}_i$ in an incremental manner. Matrix $\mathcal{S}_{i-1} \mathcal{R}_i^{-1}$ is computed via a short-term recurrence formula so that $X_{i+1} = X_i + P_i \eta_i$, where $\mathcal{S}_{i-1} \mathcal{R}_i^{-1} = [P_0, \ldots, P_i]$; we refer to [19] for a detailed description. Similar relations hold for $\tilde{R}_i$ and $\tilde{X}_i$ and thus will not be repeated here. The distance from a complete minimization procedure can be evaluated as [19]

$$\|R_i\| \le s\sqrt{i+1}\,\|R_{i,opt}\|,$$

where $R_{i,opt}$ stands for the residual of the minimum residual method.

The only cost added to the present implementation is due to the computation of the numerical rank of the approximate solutions at each step, so to stop the recurrence if the singular values of X_i or $\tilde{X}_i$ vanish.

4. Computation of the basis. Starting with a matrix $X \in \mathbb{R}^{N\times k}$, the iterative process consists of computing the vectors of the null basis of A k at the time, and then combining the new vectors with the ones already determined. In exact arithmetic and for general enough starting blocks $\tilde{X}_0, \tilde{Y}_0$, the iterative procedure ends when the rank of the computed basis is smaller than $k \cdot it$, where it is the number of cycles. In practice, however, it may be advisable to carry out an additional inner loop to prevent an underestimation of the rank. We refer to [2] for a sufficient condition on $\tilde{X}_0, \tilde{Y}_0$ that guarantees the correctness of the stopping test. If the starting guess size k is such that $k > \dim(\mathcal{N}(A))$, then the redundant vectors of the basis are deflated as soon as numerical loss of rank in the solution is detected.

The blocks of basis vectors are determined with MBBICG (cf. Section 3.1). The process continues as long as the solutions retain full rank. Otherwise, MBBICG is interrupted to deflate the unnecessary columns. We point out that in view of the properties of MBBICG, a basis for both $\mathcal{N}(A)$ and $\mathcal{N}(A^T)$ is computed, which can be required in application. The algorithm is given below.

ALGORITHM $[X, Y]$=BASIS$(A, \varepsilon, \varepsilon_1, k)$
Given $X = \emptyset, Y = \emptyset$ and $\hat{k} := k$, $k_{tot} := 0$
while (min(rank(Y), rank$(X)) = k_{tot}$)
1.1 Let $X_0, Y_0 \in \mathbb{R}^{N\times\hat{k}}$
1.2 $\tilde{X}_0 = (I - XX^T)X_0, \qquad \tilde{Y}_0 = (I - YY^T)Y_0$
2.0 $\tilde{k} = \hat{k}$
2.1 Determine Z_X, Z_Y such that

$$\max\left(\|A(Z_X + \tilde{X}_0)\|_\alpha, \|A^T(Z_Y + \tilde{Y}_0)\|_\alpha\right) \le \varepsilon$$

and stop whenever

$$\hat{k} := \min\left(\text{rank}(Z_X + \tilde{X}_0, \varepsilon_1), \text{rank}(Z_Y + \tilde{Y}_0, \varepsilon_1)\right) \ne \tilde{k}$$

2.3 $[\tilde{X}_0, \tilde{Y}_0]$ =PERM$(Z_X + \tilde{X}_0, Z_Y + \tilde{Y}_0, \hat{k})$
2.4 if $(\hat{k} \ne \tilde{k})$ and $(\hat{k} > 0)$ goto 2.0
1.4 $k_{tot} = k_{tot} + k$
1.5 $[X, Y]$ =MGS$(X, \tilde{X}_0, Y, \tilde{Y}_0, \varepsilon_1)$

The size of the null basis determined by BASIS is $\tilde{r} = \dim(\text{span}\{X\})$, or, equivalently, $\tilde{r} = \dim(\text{span}\{Y\})$. The norm $\|X\|_\alpha$ for $X \in \mathbb{R}^{N\times k}$ is defined as $\|X\|_\alpha = \sqrt{\max(\text{diag}(X^TX))}$. Steps 2.0-2.4 are repeated until a non null rank pair $Z_X + \tilde{X}_0, Z_Y + \tilde{Y}_0$ satisfying the norm tolerance is computed, producing an inner-outer type iterative procedure. We note that the outer loop is repeated only when $r \ge k$, otherwise, the algorithm ends after the inner loop.

At each iteration of MBBICG a QR decomposition with permutation matrices G_X and G_Y of the two solutions is carried out. The residuals are thus calculated on the computed orthogonal columns, rather than on the two approximate solutions. This yields a more accurate evaluation of the basis. The QR algorithm with pivoting on $X \in \mathbb{R}^{N\times\hat{k}}$ delivers a matrix $Q = [Q_1, Q_2]$ with orthogonal columns such that span$\{Q_1\}$ =span$\{X\}$ and $X = Q\rho$ where ρ is an upper triangular square matrix. Therefore, if $\|AX\|_\alpha = \delta$, then $\|AQ_1\|_\alpha \approx \delta$, whereas $\|AQ_2\|_\alpha \gg \delta$. In order to correctly monitor the full rank restriction, however, the dropping test is done by comparing the singular values of ρ_X and ρ_Y (the QR triangular factors of $Z_X + \tilde{X}_0$ and $Z_Y + \tilde{Y}_0$) with ε_1 via function rank$(\cdot, \varepsilon_1)$. A cheaper but less reliable control could be done on the diagonal elements of the triangular factors [9]. The routine PERM (line 2.3) permutes the columns of $Z_X + \tilde{X}_0, Z_Y + \tilde{Y}_0$ according to G_X and G_Y and deflates the

TABLE 5.1

*Example*1. *Detected dimension $\tilde{r}$ of the null basis, norm of optimal perturbation and true error norm for matrices A_1, A_2 and A_3 as k changes. Parameters $(\varepsilon, \varepsilon_1) = (10^{-8}, 10^{-4})$.*

	A_1			A_2			A_3		
k	$\tilde{r}$	$\|E\|_2$	$\|\mathcal{P} - \tilde{\mathcal{P}}\|_2$	$\tilde{r}$	$\|E\|_2$	$\|\mathcal{P} - \tilde{\mathcal{P}}\|_2$	$\tilde{r}$	$\|E\|_2$	$\|\mathcal{P} - \tilde{\mathcal{P}}\|_2$
1	10	4.4e-05	2.9e-06	10	2.7e-04	5.0e-06	10	4.1e-06	1.9e-04
4	10	1.9e-05	2.1e-06	10	5.1e-05	3.9e-06	10	3.4e-06	1.8e-05
8	10	9.4e-07	9.3e-08	10	1.8e-06	2.5e-08	10	1.0e-07	4.0e-05
12	10	5.3e-09	1.4e-09	10	9.1e-11	1.7e-11	10	9.6e-09	1.4e-04
16	10	9.1e-10	2.8e-10	10	4.9e-11	3.0e-11	10	1.2e-09	8.6e-07
20	10	2.6e-08	3.7e-09	10	5.8e-09	1.2e-08	10	2.3e-09	8.4e-05

last $\tilde{k} - \hat{k}$ redundant columns. If the remaining columns do not pass the convergence test, MBBICG is restarted with new blocks of rank $\hat{k}$.

Routine MGS applies a simple variant of the modified Gram-Schmidt procedure with re-orthogonalization to insert $\tilde{X}_0$ and $\tilde{Y}_0$ in the orthogonal bases X and Y. The two are carried out simultaneously, so that redundant columns of either $\tilde{X}_0$ or $\tilde{Y}_0$ can be deflated from both blocks. The main advantage of using MGS is that its cost is only due to the orthogonalization of the additional columns, while the preexisting basis remains untouched. However, it is known that the Gram-Schmidt method is less stable than other approaches when the columns of the matrix are not fairly independent [7]. The more expensive SVD on $[X, \tilde{X}_0]$ and $[Y, \tilde{Y}_0]$ or other sophisticated methods (cf. [4]) should be preferred when working with a matrix A whose smallest non-zero singular values are close to zero.

We also observe that step 1.2 is of practical little significance, since in building the Krylov subspace one computes $A^i\tilde{X}_0 = A^iX_0 - A^iX(X^TX_0)$, $i > 0$. Inthere, $A^iX = A^{i-1}(AX)$ and matrix AX has small norm. Therefore an implicit deflation is carried out and step 1.2 could be omitted. On the other hand, this shows that a necessary condition for the method to be successful is that the subsequently computed X_0, Y_0 contain components of the whole null space. Randomly generated columns usually satisfy this requirement.

The choice of the tolerances ε and ε_1 is very delicate. The parameter ε determines the maximum residual allowed on each new generated block. Nonetheless, it is always possible to check the true optimal perturbation by computing the norm of $E = E_{(0)}$ as in Theorem 2.1.

If $\sigma_{min}(A) \gg \|E\|_2$, then dim($\mathcal{N}(A)$) can be detected (cf. Corollary 2.3). Otherwise, inequality (2.1) says that a small $\sigma_{min}(A)$ may be harmful if a precise evaluation of the null basis is requested. In fact, let V be a basis for the null space of A and v be the right singular vector associated to $\sigma_{min}(A)$. Then $\|A[V, v]\|_2 = \sigma_{min}(A)$ which will be satisfactory for our purposes if $\sigma_{min}(A) < \varepsilon$. Depending on the target application, however, it may be advisable to equally consider the computed matrix $[V, v]$ as an "almost" null basis. In terms of spectrum of A, this corresponds to the problem of relatively close eigenvalues [9].

The parameter ε_1 monitors the orthogonality of the computed basis. Besides the addition of undesired vector columns, a small ε_1 may highly influence the convergence of the algorithm MBBICG in the inner loop, since the block method is very sensitive to the composition of the recurrence blocks [19].

5. Some experiments. In this section we analyze the behavior of the algorithm BASIS as the condition number of A varies. We therefore consider matrices of size $N = 100$, which differ from each other only in the last nonzero singular value.

The set of matrices was chosen so that the first, nonsingular, matrix A_0 has geometrically distributed singular values and condition number $\kappa = 100$, namely $\sigma_{N-i} = (\kappa^{\frac{-1}{N-1}})^i$ for

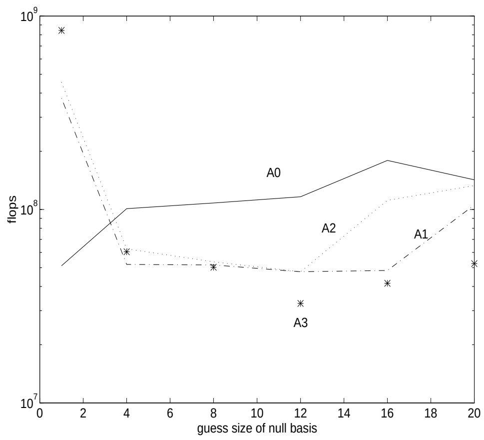

FIG. 5.1. *Floating point operations for different starting guesses for dim($\mathcal{N}(A_i)$),* $i = 0, \ldots, 3$.

$i = 0, \ldots, N-1$ [10]. This is a "tough" matrix for Krylov subspace methods, with highly indefinite symmetric part and eigenvalues λ with $|\lambda| < 1$. Due to the small size of the matrix, the SVD triples $\{u_i, \sigma_i, v_i\}_{i=1,\ldots,N}$ are readily available. In order to generate A_1, the last $r = 10$ triples $\{u_i, \sigma_i, v_i\}$ are deflated, that is $A_1 = A_0 - \sum_{i=N-r+1}^{N} u_i \sigma_i v_i^T$. This yields $\sigma_{min}(A_1) = 0.0159$ and $\sigma_1(A_1)/\sigma_{min}(A_1) \approx 62$. Matrices A_2 and A_3 are determined by subtracting the dyad from A_1 corresponding to $\sigma_{min}(A_1)$,

$$A_2 = A_1 - u_{N-r} 0.015 v_{N-r}^T, \qquad A_3 = A_1 - u_{N-r} 0.01592 v_{N-r}^T,$$

so that $\sigma_{min}(A_2) = 0.00092$ and $\sigma_{min}(A_3) = 2.8 \cdot 10^{-6}$.

In the first set of tests we compare the cost of the procedure for different values of starting block dimensions. Moreover, we monitor the norm of the minimum backward perturbation and the distance from the exact null space by using the results of the previous sections. In the second set of experiments we instead study the convergence of the algorithm for two different implementations and for several parameters selections. All experiments of this section were done using Matlab ([15]) on an SGI with machine epsilon eps=$2.2 \cdot 10^{-16}$. The matrices X_0, Y_0 (line 1.1 in the algorithm) were subsequently selected from two fixed randomly generated large matrices (matlab function `rand`). This ensures that different blocks of size k_1 and $k_2 > k_1$ differ only in the last $k_2 - k_1$ columns. The stopping test for MBBICG is given by the condition at line 2.1 in the code.

Example 1. We first analyze the method for several choices of block size k. We remark that we do not assume any a priori knowledge of the size of $\mathcal{N}(A)$. The convergence and orthogonality tolerances are fixed at $\varepsilon = 10^{-8}$ and $\varepsilon_1 = 10^{-4}$. In Figure 5.1 floating point operations count (flops) for matrices $A_0, \ldots, A_3$ is reported. For the nonsingular matrix A_0 the cost amounts to the number of operations the algorithm takes to deflate all k columns of the starting matrix. In Table 5.1 the norm of the optimal backward error E (cf. Theorem 2.1) and the distance $\|\mathcal{P} - \tilde{\mathcal{P}}\|_2$ are reported. The detected dimension of the null space is also indicated. In all cases the iterative procedure is able to correctly detect the dimension of the null space. We also observe that for a starting guess $k > r$ the norm of the optimal backward error is always smaller than for $k < r$. This, together with the cost involved in the computation (cf. Figure 5.1), suggests that it may be convenient to start the iterative procedure with a large guess k, which also justifies the use of a block method.

TABLE 5.2

$Example$2. Detected dimension $\tilde{r}$ of $\mathcal{N}(A_3)$ for different threshold values $(\varepsilon, \varepsilon_1)$. Numerical deflation with MGS.

$(\varepsilon, \varepsilon_1)$	$(10^{-8}, 10^{-4})$		$(10^{-6}, 10^{-4})$		$(10^{-6}, 10^{-6})$		$(10^{-8}, 10^{-6})$	
k	$\tilde{r}$	flops	$\tilde{r}$	flops	$\tilde{r}$	flops	$\tilde{r}$	flops
4	10	7.2e+07	13	8.1e+07	14	8.1e+07	13	9.9e+07
8	10	5.6e+07	11	4.9e+07	12	4.9e+07	11	5.6e+07
12	10	4.5e+07	10	3.2e+07	10	4.6e+07	10	4.6e+07
16	10	5.6e+07	10	4.1e+07	-	-	-	–
20	10	6.5e+07	10	5.2e+07	10	8.5e+07	10	9.8e+07

TABLE 5.3

$Example$2. Detected dimension $\tilde{r}$ of $\mathcal{N}(A_3)$ for different threshold values $(\varepsilon, \varepsilon_1)$. Numerical deflation with SVD.

$(\varepsilon, \varepsilon_1)$	$(10^{-8}, 10^{-4})$		$(10^{-6}, 10^{-4})$		$(10^{-6}, 10^{-6})$		$(10^{-8}, 10^{-6})$	
k	$\tilde{r}$	flops	$\tilde{r}$	flops	$\tilde{r}$	flops	$\tilde{r}$	flops
4	10	7.3e+07	11	6.0e+07	14	7.9e+07	10	7.3e+07
8	10	5.8e+07	11	5.0e+07	11	5.0e+07	11	5.8e+07
12	10	4.6e+07	10	3.2e+07	10	4.7e+07	10	4.7e+07
16	10	5.6e+07	10	4.1e+07	-	–	-	–
20	10	6.5e+07	10	5.2e+07	10	8.6e+07	10	9.8e+07

Example 2. We next experiment with different choices of the convergence and orthogonality tolerances ε and ε_1. In particular we compare the successful choice $(\varepsilon, \varepsilon_1) = (10^{-8}, 10^{-4})$ with other selections on the sensitive matrix A_3. Table 5.2 and Table 5.3 report the detected basis dimension and the cost for different pairs of $(\varepsilon, \varepsilon_1)$ when using MGS or an SVD for updating the null basis. A dash ('$-$') in the tables stands for lack of convergence of the inner algorithm in the iterative procedure. Note how this is sensitive to the selection of the pair $(\varepsilon, \varepsilon_1)$. It is evident that the SVD yields more accurate results, and thus less work, than the a-priori cheaper Gram-Schmidt procedure. Moreover, the total cost when the final size is the same is equivalent for the two routines. This suggests that the higher cost of the SVD is balanced by a more accurate computation.

Problems in detecting the exact dimension are mostly encountered when the tolerance approximates the smallest singular value of A_3, as expected. We can also deduce that in general a strict test with ε_1 is required. However, if the solution is sufficiently accurate, the orthogonality of the associated basis can be more easily evaluated.

6. Comments and future work. Several issues remain open. Some of them are discussed below. In some applications it is necessary to deal with a null space of large dimension which is applied by means of several subsequent matrix-matrix multiplications [6, 1]. This may become computationally expensive if the available null basis is dense. The present implementation of BASIS does not produce sparse bases. However, the analysis of some sparsity strategies would be highly desirable.

The algorithm presently requires to restart the iterative solver MBBICG every time loss of rank is detected. Instead of restarting, a dynamic deflation of the redundant columns would be preferable, since it would prevent loss of generated information. Suggested variants of block BiCG ([18]) generate additional block matrices for which a full term recurrence is required, so that their applicability is limited to the case of late deflation.

Finally, a remarkable application of the introduced technique is connected to the computation of invariant subspaces of generalized eigenvectors X such that $(A - \lambda I)^i X = 0$, $i < n$, where λ is an eigenvalue of A of multiplicity n [9], which would include the general case $\text{ind}(A) \geq 1$. Moreover, the present method could be effectively used as preconditioning strategy on quasi-singular matrices to deflate the invariant subspace corresponding to the smallest eigenvalues.

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