DEFLATED AND AUGMENTED KRYLOV SUBSPACE METHODS: BASIC FACTS AND A BREAKDOWN-FREE DEFLATED MINRES

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Abstract. In this paper we consider deflation and augmentation techniques for accelerating the convergence of Krylov subspace methods for the solution of nonsingular linear algebraic systems. The two techniques are conceptually different from preconditioning. Deflation "removes" certain parts from the operator, while augmentation adds a subspace to the Krylov subspace. Both approaches have been used in a variety of methods and settings. For Krylov subspace methods that satisfy a (Petrov-) Galerkin condition we show that augmentation can in general be achieved implicitly by projecting the residuals appropriately and correcting the approximate solutions in a final step. In this context, we analyze known methods to deflate CG, GMRES and MINRES. Our analysis reveals that the recently proposed RMINRES method can break down. We show how such breakdowns can be avoided by choosing a special initial guess, and we derive a breakdown-free deflated MINRES method. In numerical experiments we study the properties of different variants of MINRES analyzed in this paper.

Key words. Krylov subspace methods, augmentation, deflation, subspace recycling, CG, MINRES, GMRES

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1. Introduction.

Krylov subspace methods are among the most efficient tools for solving large linear algebraic systems

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{1.1}$$

where $\mathbf{A} \in \mathbb{C}^{N\times N}$ is nonsingular and $\mathbf{b} \in \mathbb{C}^N$. There exist numerous approaches to accelerate the speed of convergence of these methods. The most widely used approach is *preconditioning*, in which the system (1.1) is modified using left- and/or right-multiplications with a nonsingular matrix. The general goal of preconditioning is to obtain a modified matrix that is in some sense "close" to the identity matrix.

In this paper we consider two approaches for convergence acceleration that are different from preconditioning. The first one is *deflation*. Here one multiplies the system (1.1) with a suitably chosen projection, with the general goal to "eliminate" components that slow down convergence (e.g., small eigenvalues). Thus, the original system (1.1) is modified using a *singular* matrix, which results in a singular linear algebraic system to be solved. The second approach is *augmentation*. Here the search space of the Krylov subspace method, which is at the same time the Galerkin test space, is "enlarged" by a suitably chosen subspace that contains useful information about the problem (e.g., the linear span of approximate eigenvectors of $\mathbf{A}$).

The first deflation and augmentation techniques in the context of Krylov subspace methods appeared in the papers of Nicolaides [16] and Dostál [3]. Both proposed deflated variants of the CG method [7] to accelerate the speed of convergence for symmetric positive definite matrices $\mathbf{A}$ arising from discretized elliptic partial differential equations. Since these early works, deflation and augmentation have become widely

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used tools and have been exploited by several authors working in different fields of numerical analysis. For nonsymmetric systems Morgan [12] extracted approximate eigenvectors of $\mathbf{A}$ from the Krylov subspace produced by the GMRES method [19], and then he augmented the Krylov subspace with these vectors; for related references we refer to [6]. A comparable approach in the context of the CG method for symmetric positive definite matrices $\mathbf{A}$ was described by Saad, Yeung, Erhel, and Guyomarc'h [20]. In [9] Kolotilina used a twofold deflation technique for simultaneously deflating the r largest and the r smallest eigenvalues by an appropriate deflating subspace of dimension r. An analysis of acceleration strategies (including augmentation) for minimal residual methods was given by Saad [18] and for restarted methods by Eiermann, Ernst and Schneider [4].

In addition to deflation/augmentation spaces based on approximative eigenvectors, other choices have been studied. Mansfield [10] showed how Schur complement-type domain decomposition methods can be seen as a series of deflations. Nicolaides [16] construced a deflation technique based on piecewise constant interpolation from a set of r subdomains, and he pointed out that deflation might be effectively used with a conventional preconditioner. In [11] Mansfield used the same "subdomain deflation" in combination with damped Jacobi smoothing, and obtained a preconditioner that is related to the two-grid method.

In [13, 14, 15] Nabben and Vuik described similarities between the deflation approach and domain decomposition methods. This comparison was extended in [22, 21]. In these papers comparison results are given for arbitrary deflation spaces.

As indicated by this brief survey, deflation and augmentation can be applied to every Krylov subspace method. This resulted in a large variety of different methods and implementations. The main goal of this paper is not to add further examples to the existing collection (although we derive one apparently new method in the end), but to mathematically characterize a number of different approaches. We focus on Krylov subspace methods whose residuals satisfy a certain (Petrov-) Galerkin condition and show in what sense deflation and augmentation are mathematically equivalent (Section 2). We then discuss known approaches to deflate CG (Section 3), GMRES (Section 4), and MINRES (Section 5) in the light of our general equivalence theorem. Among other results, this will reveal that a recent version of deflated MINRES, suggested in [23] under the name RMINRES ("recycling MINRES") can break down. Based on our theoretical results we can give a modified version of this method, which cannot break down (in exact arithmetic). We do not focus on specific implementations and algorithmic details but on the mathematical theory of these methods. For the numerical application of the methods we draw on the most robust implementations of CG, MINRES and GMRES that are available.

2. A framework for deflated and augmented Krylov methods. In this section we describe a general framework for deflation and augmentation, which simultaneously covers several Krylov subspace methods whose residuals satisfy a Galerkin condition. Given an initial guess $\mathbf{x}_0 \in \mathbb{C}^N$, a positive integer n, an n-dimensional subspace $\mathcal{S}_n$ of $\mathbb{C}^N$, and a nonsingular matrix $\mathbf{B} \in \mathbb{C}^{N\times N}$, we consider an approximation $\mathbf{x}_n$ to the solution $\mathbf{x}$ of the form

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{S}_n, \tag{2.1}$$

so that the corresponding residual satisfies

$$\mathbf{r}_n := \mathbf{b} - \mathbf{A}\mathbf{x}_n \perp \mathbf{B}\mathcal{S}_n. \tag{2.2}$$

If the search space $\mathcal{S}_n$ is the nth Krylov subspace generated by $\mathbf{A}$ and the initial residual $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$, i.e., if $\mathcal{S}_n = \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0) := \text{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots \mathbf{A}^{n-1}\mathbf{r}_0\}$, then (2.1)–(2.2) mathematically characterize the CG method [7] when $\mathbf{A}$ is hpd and $\mathbf{B} = \mathbf{I}$. If $\mathbf{B} = \mathbf{A}$, and $\mathbf{A}$ is hermitian or general (nonsingular), then (2.1)–(2.2) mathematically characterize the methods MinRes [17] or GMRes [19], respectively.

Instead of a search space of the form $\mathcal{S}_n = \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ we consider here an *augmented* Krylov subspace generated by a matrix $\widehat{\mathbf{A}}$ that we consider as a *deflated* version of $\mathbf{A}$ and by the corresponding initial residual $\widehat{\mathbf{r}}_0$. For the moment, we let $\widehat{\mathbf{A}} \in \mathbb{C}^{N\times N}$ (possibly singular) and $\widehat{\mathbf{r}}_0 \in \mathbb{C}^N$ be arbitrary, except for the requirement that the Krylov subspace $\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$ has dimension n. Examples for choices of $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{r}}_0$ that result in practical methods will be discussed in the later sections.

So, the augmented Krylov subspace is of the form

$$\mathcal{S}_n := \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U}, \tag{2.3}$$

where $\mathcal{U}$ is the so-called *augmentation space*. We suppose that $\mathcal{U}$ has dimension k, and denote by $\mathbf{U} \in \mathbb{C}^{N\times k}$ a matrix whose columns form a basis of $\mathcal{U}$. Using this matrix and a matrix $\mathbf{V}_n \in \mathbb{C}^{N\times n}$ whose columns form a basis of $\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$, (2.1) can be written as

$$\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n + \mathbf{U}\mathbf{u}_n \tag{2.4}$$

for some vectors $\mathbf{y}_n \in \mathbb{C}^n$ and $\mathbf{u}_n \in \mathbb{C}^k$. Of course, $\mathbf{U}$ may be redefined when an algorithm like GMRes is restarted, but we will not account for that in our notation.

In order to satisfy (2.2), the residual $\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ must be orthogonal to both $\mathbf{B}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$ and $\mathbf{B}\mathcal{U}$, which means that it must satisfy the pair of orthogonality conditions

$$\mathbf{r}_n \perp \mathbf{B}\,\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) \quad \text{and} \quad \mathbf{r}_n \perp \mathbf{B}\,\mathcal{U}. \tag{2.5}$$

Let us concentrate on the second condition, which in matrix-form can be written as

$$\mathbf{0} = \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{r_n} = \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\left(\mathbf{r_0} - \mathbf{A}\mathbf{V_n}\mathbf{y_n} - \mathbf{A}\mathbf{U}\mathbf{u_n}\right) = \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\left(\mathbf{r_0} - \mathbf{A}\mathbf{V_n}\mathbf{y_n}\right) - \mathbf{E_B}\mathbf{u_n},$$

where

$$\mathbf{E_B} := \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}\mathbf{U} \in \mathbb{C}^{k\times k}. \tag{2.6}$$

In the following, a general requirement will be that the matrix $\mathbf{E_B}$ is nonsingular. We will discuss cases where this is satisfied in subsequent sections. If $\mathbf{E_B}$ is nonsingular, then the second orthogonality condition is equivalent to

$$\mathbf{u}_n = \mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n\right). \tag{2.7}$$

Using this in (2.4) gives

$$\begin{aligned}
\mathbf{x}_n &= \mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n + \mathbf{U}\left(\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n\right)\right) \\
&= \left(\mathbf{I} - \mathbf{U}\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}\right)\left(\mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n\right) + \mathbf{U}\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{b}, \qquad (2.8) \\
\mathbf{r}_n &= \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n - \mathbf{A}\mathbf{U}\left(\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n\right)\right) \\
&= \left(\mathbf{I} - \mathbf{A}\mathbf{U}\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\right)\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n\right). \qquad (2.9)
\end{aligned}$$

To simplify the notation we define the $(N \times N)$-matrices

$$\begin{aligned} \mathbf{Q_B} &:= \mathbf{U}\mathbf{E_B}^{-1}\mathbf{U}^{\mathsf{H}} = \mathbf{U}\left(\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}\mathbf{U}\right)^{-1}\mathbf{U}^{\mathsf{H}}, \\ \mathbf{P_B} &:= \mathbf{I} - \mathbf{A}\mathbf{Q_B}\mathbf{B}^{\mathsf{H}}, \\ \widetilde{\mathbf{P}}_{\mathbf{B}} &:= \mathbf{I} - \mathbf{Q_B}\mathbf{B}^{\mathsf{H}}\mathbf{A}. \end{aligned} \tag{2.10}$$

We next state some basic properties of the matrices $\mathbf{P_B}$ and $\widetilde{\mathbf{P}}_{\mathbf{B}}$. The proof of these properties is straightforward, and is therefore omitted.

LEMMA 2.1.

1. $\mathbf{P_B}^2 = \mathbf{P_B}$, $\mathbf{P_B}\mathbf{A}\mathbf{U} = \mathbf{0}$, *and* $\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{P_B} = \mathbf{0}$, *i.e.,* $\mathbf{P_B}$ *is the projection onto* $(\mathbf{B}\mathcal{U})^{\perp}$ *along* $\mathbf{A}\mathcal{U}$.
2. $\widetilde{\mathbf{P}}_{\mathbf{B}}^2 = \widetilde{\mathbf{P}}_{\mathbf{B}}$, $\widetilde{\mathbf{P}}_{\mathbf{B}}\mathbf{U} = \mathbf{0}$, *and* $\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}\widetilde{\mathbf{P}}_{\mathbf{B}} = \mathbf{0}$, *i.e.,* $\widetilde{\mathbf{P}}_{\mathbf{B}}$ *is the projection onto* $\left(\mathbf{A}^{\mathsf{H}}\mathbf{B}\mathcal{U}\right)^{\perp}$ *along* $\mathcal{U}$.
3. $\mathbf{P_B}\mathbf{A} = \mathbf{A}\widetilde{\mathbf{P}}_{\mathbf{B}}$.

Using the matrices defined in (2.10), the equations (2.8) and (2.9) take the form

$$\mathbf{x}_n = \widetilde{\mathbf{P}}_{\mathbf{B}}\left(\mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n\right) + \mathbf{Q_B}\mathbf{B}^{\mathsf{H}}\mathbf{b}, \tag{2.11}$$

$$\mathbf{r}_n = \mathbf{P_B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{y}_n\right) \tag{2.12}$$

Note that imposing the second orthogonality condition in (2.5) on the residual $\mathbf{r}_n$ has determined the vector $\mathbf{u}_n$, which has therefore "disappeared" in (2.11)–(2.12).

It remains to impose the first orthogonality condition in (2.5), which will determine the vector $\mathbf{y}_n$. To this end, let

$$\widetilde{\mathbf{x}}_n := \mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0),$$

then $\mathbf{x}_n = \widetilde{\mathbf{P}}_{\mathbf{B}}\widetilde{\mathbf{x}}_n + \mathbf{Q_B}\mathbf{B}^{\mathsf{H}}\mathbf{b}$. Using the definition of $\mathbf{P_B}$ in (2.10) and Condition 3 from Lemma 2.1, the orthogonality condition becomes

$$\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n = \mathbf{P_B}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) \perp \mathbf{B}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0).$$

We summarize these considerations in the following theorem.

THEOREM 2.2. *Using the previous notation, the following two sets of conditions,*

$$\begin{aligned} &\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U}, \\ &\mathbf{r}_n := \mathbf{b} - \mathbf{A}\mathbf{x}_n \perp \mathbf{B}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathbf{B}\mathcal{U}, \end{aligned} \tag{2.13}$$

and

$$\begin{aligned} &\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0), \\ &\widetilde{\mathbf{r}}_n := \mathbf{P_B}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) \perp \mathbf{B}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0). \end{aligned} \tag{2.14}$$

are equivalent for $n \geq 1$ *in the sense that*

$$\mathbf{x}_n = \widetilde{\mathbf{P}}_{\mathbf{B}}\widetilde{\mathbf{x}}_n + \mathbf{Q_B}\mathbf{B}^{\mathsf{H}}\mathbf{b}, \quad \textit{and} \quad \mathbf{r}_n = \widetilde{\mathbf{r}}_n. \tag{2.15}$$

Note that $\widehat{\mathbf{A}}$ and $\mathcal{U}$ are in general unrelated. The conditions (2.13) represent the standard augmentation approach, where the augmentation space $\mathcal{U}$ is explicitly included in the search space. The equivalent conditions (2.14) show that the explicit inclusion of $\mathcal{U}$ can be omitted when instead we first construct the iterate

$\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$ so that the "projected residual" $\widetilde{\mathbf{r}}_n = \mathbf{P_B}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n)$ satisfies the given orthogonality condition and then apply the affine correction (2.15) to $\widetilde{\mathbf{x}}_n$, whose projected residual equals the one of $\mathbf{x}_n$.

So far we have not specified the matrix $\widehat{\mathbf{A}}$ and the vector $\widehat{\mathbf{r}}_0$. In the following sections we will discuss suitable choices for $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{r}}_0$ that depend on the properties of the matrix $\mathbf{A}$.

3. Hermitian positive definite matrices and CG. Throughout this section we assume that $\mathbf{A}$ is hpd. We choose $\mathbf{B} = \mathbf{I}$ and some k-dimensional augmentation space $\mathcal{U}$ with the corresponding matrix $\mathbf{U}$. Then the matrix $\mathbf{E_I} = \mathbf{U}^\mathsf{H}\mathbf{A}\mathbf{U}$ is nonsingular, and thus our general requirement is satisfied; cf. (2.6)–(2.7).

We use the matrix $\mathbf{U}$ and the definitions from (2.10) to set up the *deflated system*

$$\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}, \quad \text{where} \quad \widehat{\mathbf{A}} := \mathbf{P_I}\mathbf{A}, \quad \widehat{\mathbf{b}} := \mathbf{P_I}\mathbf{b}. \tag{3.1}$$

Hence the deflated system results from a left-multiplication of the given system $\mathbf{A}\mathbf{x} = \mathbf{b}$ with the projection

$$\mathbf{P_I} = \mathbf{I} - \mathbf{A}\mathbf{U}(\mathbf{U}^\mathsf{H}\mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\mathsf{H},$$

which projects onto $\mathcal{U}^\perp$ along $\mathbf{A}\mathcal{U}$. In the context of hpd matrices and the CG method this is a commonly used technique; see, e.g., [22] for a survey of results. Clearly, the deflated matrix $\widehat{\mathbf{A}}$ is hermitian and nonzero, but singular, since $\mathbf{P_I}$ is a nontrivial projection if $0 < k < N$. We point out that $\widehat{\mathbf{A}}$ as defined in (3.1) is completely determined by $\mathbf{A}$ and the choice of the augmentation space $\mathcal{U}$. (Recall that in Theorem 2.2 the matrix $\widehat{\mathbf{A}}$ and the subspace $\mathcal{U}$ can be unrelated.)

According to Nicolaides [16] and Kaasschieter [8], the CG method is well defined (in exact arithmetic) for each step n until it terminates with the exact solution, when it is applied to a consistent linear algebraic system with a real and symmetric positive semidefinite matrix. This result easily generalizes to complex and hermitian positive semidefinite matrices.

In our case the system (3.1) is consistent since it results from a left-multiplication of the consistent system $\mathbf{A}\mathbf{x} = \mathbf{b}$ with $\mathbf{P_I}$. We have already noted above that $\widehat{\mathbf{A}}$ is hermitian, and this matrix is also positive semi-definite, since

$$\mathbf{v}^\mathsf{H}\widehat{\mathbf{A}}\mathbf{v} = \mathbf{v}^\mathsf{H}\mathbf{P_I}\mathbf{A}\mathbf{v} = \mathbf{v}^\mathsf{H}\mathbf{P_I}^2\mathbf{A}\mathbf{v} = \mathbf{v}^\mathsf{H}\mathbf{P_I}(\mathbf{P_I}\mathbf{A})\mathbf{v} = \mathbf{v}^\mathsf{H}\mathbf{P_I}(\mathbf{P_I}\mathbf{A})^\mathsf{H}\mathbf{v} = \mathbf{v}^\mathsf{H}\mathbf{P_I}\mathbf{A}\mathbf{P_I}^\mathsf{H}\mathbf{v} \geq 0$$

holds for any $\mathbf{v} \in \mathbb{C}^N$.

Mathematically, the nth step of the CG method applied to the deflated system (3.1) with the initial guess $\mathbf{x}_0$ and the resulting initial residual $\widehat{\mathbf{r}}_0 = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\mathbf{x_0}$ is characterized by the two conditions

$$\begin{aligned}
&\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0),\\
&\widetilde{\mathbf{r}}_n = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widetilde{\mathbf{x}}_n = \mathbf{P_I}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) \perp \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0).
\end{aligned}$$

This is nothing but the set of conditions (2.14) with $\mathbf{B} = \mathbf{I}$. In the sense of relation (2.15) these conditions have been shown to be equivalent to (2.13), namely

$$\begin{aligned}
&\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U},\\
&\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n \perp \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U}.
\end{aligned}$$

This is the starting point of the deflated CG method developed in [20].

The goal is to obtain a deflated matrix $\widehat{\mathbf{A}}$ whose effective condition number is smaller than the one of $\mathbf{A}$, for example by "eliminating" the smallest eigenvalues of $\mathbf{A}$. A detailed analysis of spectral properties of $\mathbf{P_I A}$ for different projections arising from domain decomposition and multigrid methods was carried out in [14] and [22]. In particular, it was shown in these papers that the effective condition number of $\widehat{\mathbf{A}}$ is less than or equal to the condition number of $\mathbf{A}$ for *any* augmentation space $\mathcal{U}$. Moreover, if $\mathcal{U}$ is an $\mathbf{A}$-invariant subspace, the corresponding eigenvalues do not count for this effective condition number of $\widehat{\mathbf{A}}$.

In summary, for *any* augmentation space $\mathcal{U}$, the CG method applied to the (singular) deflated system (3.1) is well defined for any iteration step n, and it terminates with an exact solution $\widehat{\mathbf{x}}$ (in exact arithmetic). This computation is mathematically equivalent to an explicit use of augmentation. Once CG has terminated with a solution $\widehat{\mathbf{x}}$ of the deflated system, we can obtain the uniquely defined solution of the original system using the final correction step

$$\mathbf{x} = \widetilde{\mathbf{P}}_\mathbf{I}\widehat{\mathbf{x}} + \mathbf{Q_I b}$$

(cf. (2.15)), which indeed gives

$$\mathbf{Ax} = \mathbf{A}\widetilde{\mathbf{P}}_\mathbf{I}\widehat{\mathbf{x}} + \mathbf{AQ_I b} = \mathbf{P_I A}\widehat{\mathbf{x}} + \mathbf{AQ_I b} = (\mathbf{P_I} + \mathbf{AQ_I})\mathbf{b} = \mathbf{b}.$$

Of course, in practice we stop the CG iteration for the deflated system once the solution is appoximated sufficiently accurately. We then use the computed approximation $\widehat{\mathbf{x}}_n$ and (2.15) to obtain an approximation $\mathbf{x}_n$ of the solution of the given system $\mathbf{Ax} = \mathbf{b}$. Note that, according to (2.15), the residual $\widehat{\mathbf{r}}_n = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widehat{\mathbf{x}}_n$ of the projected system (3.1) is equal to the residual $\mathbf{r}_n = \mathbf{b} - \mathbf{Ax}_n$ of the original system (1.1).

4. Non-hermitian matrices and GMRES**.** In this section we consider a general nonsingular matrix $\mathbf{A}$, and $\mathbf{B} = \mathbf{A}$. A similar situation has been considered by Morgan [12] and also Chapman and Saad [2]. They presented variations of GMRES that can be mathematically described by (2.13) with $\widehat{\mathbf{A}} = \mathbf{A}$ and $\widehat{\mathbf{r}}_0 = \mathbf{b} - \mathbf{Ax}_0$; that is, they augmented the bases but did not deflate the matrix and project the linear system into a subspace of $\mathbb{C}^N$.

Erlangga and Nabben [5] used two deflation matrices $\mathbf{Y}, \mathbf{Z}$ for non-hermitian matrices $\mathbf{A}$. The resulting deflation technique is similar to the choice of $\mathbf{B} = \mathbf{I}$ in our setting. However, this choice needs the assumption of nonsingularity of $\mathbf{Y}^\mathsf{H}\mathbf{AZ}$.

Here, we will consider a different approach. If $\mathbf{B} = \mathbf{A}$, then the matrix $\mathbf{E_A} = \mathbf{U}^\mathsf{H}\mathbf{A}^\mathsf{H}\mathbf{AU}$ is nonsingular for any (nontrivial) augmentation space $\mathcal{U}$, so that again our general requirement is satisfied; see (2.6)–(2.7). Analogously to the approach for CG described in the previous section, we deflate the given system $\mathbf{Ax} = \mathbf{b}$ by a left-multiplication with

$$\mathbf{P_A} = \mathbf{I} - \mathbf{AQ_A}\mathbf{A}^\mathsf{H} = \mathbf{I} - \mathbf{AU}(\mathbf{U}^\mathsf{H}\mathbf{A}^\mathsf{H}\mathbf{AU})^{-1}\mathbf{U}^\mathsf{H}\mathbf{A}^\mathsf{H},$$

which projects onto $(\mathbf{A}\mathcal{U})^\perp$ along $\mathbf{A}\mathcal{U}$. Note that this is an orthogonal projection, and consequently $\mathbf{P_A}$ is hermitian.

We now consider the application of GMRES to the deflated system

$$\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}, \quad \text{where} \quad \widehat{\mathbf{A}} := \mathbf{P_A A}, \quad \widehat{\mathbf{b}} := \mathbf{P_A b}. \tag{4.1}$$

If we start GMRES with an initial guess $\mathbf{x}_0$ and the corresponding initial residual $\widehat{\mathbf{r}}_0 = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\mathbf{x}_0 = \mathbf{P_A}(\mathbf{b} - \mathbf{Ax}_0)$, then the iterate $\widetilde{\mathbf{x}}_n$ and the residual $\widetilde{\mathbf{r}}_n$ are characterized by the two conditions

$$\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0), \quad \text{and} \quad \widetilde{\mathbf{r}}_n = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widetilde{\mathbf{x}}_n \perp \widehat{\mathbf{A}}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0).$$

If the columns of $\mathbf{V}_n$ form a basis of $\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$, then the second condition means that

$$\begin{aligned}\mathbf{0} &= \mathbf{V}_n^{\mathsf{H}}\widehat{\mathbf{A}}^{\mathsf{H}}\widetilde{\mathbf{r}}_n = \mathbf{V}_n^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}_{\mathbf{A}}^{\mathsf{H}}\widetilde{\mathbf{r}}_n = \mathbf{V}_n^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}_{\mathbf{A}}\mathbf{P}_{\mathbf{A}}\left(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n\right) = \mathbf{V}_n^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}_{\mathbf{A}}\left(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n\right) \\ &= \mathbf{V}_n^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{r}}_n,\end{aligned}$$

or, equivalently,

$$\widetilde{\mathbf{r}}_n \perp \mathbf{A}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0).$$

Note that here the Krylov subspace is multiplied with $\mathbf{A}$ instead of $\widehat{\mathbf{A}}$ and that this condition has precisely the form of the second condition in (2.14). Theorem 2.2 now implies that the mathematical characterization of GMRES applied to the deflated system $\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}$ is equivalent to the explicit use of augmentation, i.e., the conditions

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U}, \tag{4.2}$$

$$\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n \perp \mathbf{A}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathbf{A}\mathcal{U}, \tag{4.3}$$

in the sense that

$$\mathbf{x}_n = \widetilde{\mathbf{P}}_{\mathbf{A}}\widetilde{\mathbf{x}}_n + \mathbf{Q}_{\mathbf{A}}\mathbf{A}^{\mathsf{H}}\mathbf{b}, \quad \text{and} \quad \mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widetilde{\mathbf{x}}_n = \widetilde{\mathbf{r}}_n. \tag{4.4}$$

Again the deflated matrix $\widehat{\mathbf{A}}$ is singular if $\mathcal{U} \neq \{\mathbf{0}\}$, and we have to discuss whether the application of GMRES to the deflated system yields (in exact arithmetic) a well defined sequence of iterates that terminates with a solution. This turns out to be significantly more difficult than in the case of the CG method. Properties of GMRES applied to singular systems have been analyzed by Brown and Walker [1], and the following result is an extension of their Theorem 2.6.

THEOREM 4.1. *Consider an arbitrary matrix $\widehat{\mathbf{A}} \in \mathbb{C}^{N\times N}$ and a vector $\widehat{\mathbf{b}} \in \mathsf{Im}\,(\widehat{\mathbf{A}})$ (i.e., the linear algebraic system $\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}$ is consistent). Then the following two conditions are equivalent:*

1. *For each initial guess $\mathbf{x}_0 \in \mathbb{C}^N$ the* GMRES *method applied to the system $\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}$ is well defined at each iteration step n and it terminates with a solution of the system.*
2. $\mathsf{ker}\,(\widehat{\mathbf{A}}) \cap \mathsf{Im}\,(\widehat{\mathbf{A}}) = \{\mathbf{0}\}$.

Proof. It has been shown in [1, Theorem 2.6] that Condition 2 implies Condition 1. We prove the reverse by contradiction. We assume that $\mathsf{ker}\,(\widehat{\mathbf{A}}) \cap \mathsf{Im}\,(\widehat{\mathbf{A}}) \neq \{\mathbf{0}\}$, and we will construct an initial guess for which GMRES does not terminate with the solution. For a nonzero vector $\mathbf{y} \in \mathsf{ker}\,(\widehat{\mathbf{A}}) \cap \mathsf{Im}\,(\widehat{\mathbf{A}})$ there exists a nonzero vector $\widehat{\mathbf{y}} \in \mathbb{C}^N$, such that $\mathbf{y} = \widehat{\mathbf{A}}\widehat{\mathbf{y}}$, and since $\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}$ is consistent, there exists a vector $\widehat{\mathbf{x}} \in \mathbb{C}^N$ with $\widehat{\mathbf{b}} = \widehat{\mathbf{A}}\widehat{\mathbf{x}}$. Then the initial guess $\mathbf{x}_0 := \widehat{\mathbf{x}} - \widehat{\mathbf{y}}$ gives $\mathbf{r}_0 = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\mathbf{x}_0 = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widehat{\mathbf{x}} + \widehat{\mathbf{A}}\widehat{\mathbf{y}} = \mathbf{y}$. But since $\mathbf{y} \in \mathsf{ker}\,(\widehat{\mathbf{A}})$, we obtain $\widehat{\mathbf{A}}\mathbf{r}_0 = \mathbf{0}$, so that the GMRES method terminates at the first iteration with the approximation $\mathbf{x}_0$, for which $\mathbf{r}_0 = \mathbf{y} \neq \mathbf{0}$. Thus, for this particular initial guess $\mathbf{x}_0$ the GMRES method cannot determine the solution of $\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}$. ∎

We next have a closer look at Condition 2 in Theorem 4.1. If we had $\mathsf{ker}\,(\widehat{\mathbf{A}}) = \mathsf{ker}\,(\widehat{\mathbf{A}}^{\mathsf{H}})$, then $\mathsf{Im}\,(\widehat{\mathbf{A}})^{\perp} = \mathsf{ker}\,(\widehat{\mathbf{A}}^{\mathsf{H}})$ would imply

$$\{\mathbf{0}\} = \mathsf{Im}\,(\widehat{\mathbf{A}})^{\perp} \cap \mathsf{Im}\,(\widehat{\mathbf{A}}) = \mathsf{ker}\,(\widehat{\mathbf{A}}^{\mathsf{H}}) \cap \mathsf{Im}\,(\widehat{\mathbf{A}}) = \mathsf{ker}\,(\widehat{\mathbf{A}}) \cap \mathsf{Im}\,(\widehat{\mathbf{A}}),$$

so that Condition 2 would hold. For a general non-hermitian matrix, however, it seems difficult to determine a deflated matrix with $\mathsf{ker}\,(\widehat{\mathbf{A}}) = \mathsf{ker}\,(\widehat{\mathbf{A}}^{\mathsf{H}})$. Nevertheless,

Theorem 4.1 gives a useful necessary and sufficient condition for the validity of the deflation approach in the context of the GMRES method.

COROLLARY 4.2. *Consider the deflated system (4.1). Then Condition 1 in Theorem 4.1 is satisfied if and only if* $\mathcal{U} \cap (\mathbf{A}\mathcal{U})^{\perp} = \{\mathbf{0}\}$. *In particular, the latter condition is satisfied when* $\mathcal{U}$ *is an exact* $\mathbf{A}$*-invariant subspace, i.e., when* $\mathbf{A}\mathcal{U} = \mathcal{U}$.

Proof. Using the properties of the projection $\mathbf{P_A}$ from Lemma 2.1 and the fact that $\mathbf{A}$ is nonsingular, we obtain

$$\begin{aligned} \mathsf{ker}\,(\widehat{\mathbf{A}}) &= \mathsf{ker}\,(\mathbf{P_A}\mathbf{A}) = \mathbf{A}^{-1}\mathsf{ker}\,(\mathbf{P_A}) = \mathcal{U}, \\ \mathsf{Im}\,(\widehat{\mathbf{A}}) &= \mathsf{Im}\,(\mathbf{P_A}\mathbf{A}) = \mathsf{Im}\,(\mathbf{P_A}) = (\mathbf{A}\mathcal{U})^{\perp}, \end{aligned}$$

and the result now follows from Theorem 4.1. If $\mathbf{A}\mathcal{U} = \mathcal{U}$, then $\mathcal{U} \cap (\mathbf{A}\mathcal{U})^{\perp} = \{\mathbf{0}\}$ holds trivially. ∎

The situation that the GMRES method terminates without having found the exact solution is often called a *breakdown* of GMRES. Such breakdown can only occur when GMRES is applied to a linear algebraic system with a singular matrix, since for a nonsingular matrix Condition 2 in Theorem 4.1 always holds. To illustrate the problem of breakdowns in our context, we give an example that is adapted from [1].

EXAMPLE 4.3. Consider a linear algebraic system with

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

so that the unique solution is given by the vector $[0, 1]^{\mathsf{T}}$. Let the augmentation space be defined by $\mathbf{U}_1 = [1, 0]^{\mathsf{T}}$, then

$$\mathbf{P_A} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \widehat{\mathbf{A}} = \mathbf{P_A}\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \widehat{\mathbf{b}} = \mathbf{P_A}\mathbf{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

If $\mathbf{x}_0$ is the zero vector, then $\widehat{\mathbf{r}}_0 = \widehat{\mathbf{b}}$ and $\widehat{\mathbf{A}}\widehat{\mathbf{r}}_0 = \mathbf{0}$, and thus GMRES applied to the deflated system terminates at the very first iteration with the approximation $\mathbf{x}_0$. Since $\widehat{\mathbf{A}}\mathbf{x}_0 \neq \widehat{\mathbf{b}}$, this is a breakdown of GMRES. Furthermore, applying the correction (2.11) to $\widetilde{\mathbf{x}}_0 = \mathbf{x}_0$ does not yield the solution of the original system $\mathbf{A}\mathbf{x} = \mathbf{b}$ because

$$\widetilde{\mathbf{P}}_{\mathbf{A}}\mathbf{x}_0 + \mathbf{Q_A}\mathbf{A}^{\mathsf{H}}\mathbf{b} = \mathbf{Q_A}\mathbf{A}^{\mathsf{H}}\mathbf{b} = \mathbf{U}_1\mathbf{U}_1^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{b} = \mathbf{0} \neq \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

5. Hermitian matrices and variants of MINRES. We will now apply the results of Sections 2 and 4 to the case where $\mathbf{A}$ is hermitian, nonsingular, and possibly indefinite. As in Section 4, we consider the choice $\mathbf{B} = \mathbf{A}$ and the resulting deflated system of the form (4.1),

$$\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{b}}, \quad \text{where} \quad \widehat{\mathbf{A}} := \mathbf{P_A}\mathbf{A}, \quad \widehat{\mathbf{b}} := \mathbf{P_A}\mathbf{b}.$$

5.1. The RMINRES method. For a hermitian matrix the GMRES method considered in Section 4 is mathematically equivalent to the MINRES method, which is based on the hermitian Lanczos algorithm, and thus uses efficient three-term recurrences. If we start MINRES with an initial guess $\mathbf{x}_0$ and the corresponding initial residual $\widehat{\mathbf{r}}_0 = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\mathbf{x}_0 = \mathbf{P_A}(\mathbf{b} - \mathbf{A}\mathbf{x}_0)$, then the iterate $\widetilde{\mathbf{x}}_n$ and the residual $\widetilde{\mathbf{r}}_n$ are characterized by the two conditions

$$\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0), \quad \text{and} \quad \widetilde{\mathbf{r}}_n = \widehat{\mathbf{b}} - \widehat{\mathbf{A}}\widetilde{\mathbf{x}}_n \perp \widehat{\mathbf{A}}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0). \tag{5.1}$$

An attentive reader certainly has noticed that the deflated matrix $\widehat{\mathbf{A}} = \mathbf{P_A A} = \mathbf{A} - \mathbf{A Q_A A}^2$ is in general *not* hermitian, even when $\mathbf{A}$ is hermitian. However, since $\mathbf{P_A}$ is a projection, a straightforward computation shows that

$$\mathcal{K}_n(\mathbf{P_A A}, \mathbf{P_A v}) = \mathcal{K}_n(\mathbf{P_A A P_A}, \mathbf{P_A v}) \tag{5.2}$$

holds for every vector $\mathbf{v} \in \mathbb{C}^N$. The matrix $\mathbf{P_A A P_A}$ is obviously hermitian (since $\mathbf{A}$ and $\mathbf{P_A}$ are hermitian), and hence the Krylov subspaces we work with are also generated by a hermitian matrix. It is therefore possible to implement a MinRes-like method for the deflated system, which is based on three-term recurrences and which is characterized by the conditions (5.1). As shown in Section 4, these conditions combined with the correction step (4.4) are equivalent to the explicit use of augmentation, i.e., conditions (4.2)–(4.3).

The latter conditions are the basis of the approach of Wang, de Sturler and Paulino in [23]. They were interested in solving sequences of nearby linear algebraic systems, and they suggested to reuse information from previous solves. More specifically, they determined harmonic Ritz vectors that correspond to harmonic Ritz values close to zero, and used these approximate eigenspaces for augmenting the Krylov subspace (which have been shown here to be equivalent to solving the deflated system). Their resulting method is called "recycling MinRes", or briefly RMinRes. Here, we omit the extraction of the augmentation space and concentrate on the method for solving the systems.

We summarize the above and give two mathematically equivalent characterizations of RMinRes applied to the system $\mathbf{Ax} = \mathbf{b}$ with initial guess $\mathbf{x}_0$:

1. The original approach used in [23] incorporates explicit augmentation, which means to construct iterates $\mathbf{x}_n$ satisfying the two conditions

$$\begin{aligned} &\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\mathbf{P_A A}, \mathbf{P_A r}_0) + \mathcal{U}, \\ &\mathbf{r}_n = \mathbf{b} - \mathbf{A x}_n \perp \mathbf{A}\mathcal{K}_n(\mathbf{P_A A}, \mathbf{P_A r}_0) + \mathbf{A}\mathcal{U}. \end{aligned} \tag{5.3}$$

2. A mathematically equivalent approach is to apply MinRes to the deflated system

$$\mathbf{P_A A x} = \mathbf{P_A b} \tag{5.4}$$

and correct the resulting iterates $\widetilde{\mathbf{x}}_n$ according to $\mathbf{x}_n = \widetilde{\mathbf{P}}_\mathbf{A} \widetilde{\mathbf{x}}_n + \mathbf{Q_A A b}$.

The RMinRes method as presented in [23] involves some interesting algorithmic details. For example, the matrix $\mathbf{U}$ is modified using a QR factorization such that $\mathbf{Z}_k := \mathbf{AU}$ is unitary, i.e., $\mathbf{Z}_k^\mathsf{H}\mathbf{Z}_k = \mathbf{I}_k$, and then $\mathbf{P_A}$ simplifies to

$$\mathbf{P_A} = \mathbf{I} - \mathbf{AU}\left(\mathbf{U}^\mathsf{H}\mathbf{A}^\mathsf{H}\mathbf{AU}\right)^{-1}\mathbf{U}^\mathsf{H}\mathbf{A}^\mathsf{H} = \mathbf{I} - \mathbf{Z}_k\left(\mathbf{Z}_k^\mathsf{H}\mathbf{Z}_k\right)^{-1}\mathbf{Z}_k^\mathsf{H} = \mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^\mathsf{H}.$$

Since RMinRes is mathematically equivalent to MinRes (and GMRes) applied to the deflated system, Corollary 4.2 also applies to RMinRes. In particular, the method can break down for specific initial guesses if (and only if) $\mathcal{U} \cap (\mathbf{A}\mathcal{U})^\perp \neq \{\mathbf{0}\}$. Breakdowns cannot occur if $\mathcal{U}$ is an exact $\mathbf{A}$-invariant subspace, but this is an unrealistic assumption in practical applications. Note that the matrix $\mathbf{A}$ in Example 4.3 is hermitian, thus it also serves as an example for a breakdown of RMinRes. In the next subsection we will show how to suitably modify the RMinRes approach to get a breakdown-free deflated MinRes solver.

5.2. Deflated MinRes without breakdowns. We have seen above, that if $\ker(\widehat{\mathbf{A}}) = \ker(\widehat{\mathbf{A}}^{\mathsf{H}})$, then Condition 1 in Theorem 4.1 is satisfied. Consequently, if we can determine a *hermitian deflated matrix* $\widehat{\mathbf{A}}$ and a corresponding consistent deflated system, MinRes applied to this system cannot break down for any initial guess.

Using the projections $\mathbf{P_A}$ and $\widetilde{\mathbf{P}}_\mathbf{A}$ from (2.10) we decompose the solution $\mathbf{x}$ of $\mathbf{Ax} = \mathbf{b}$ as

$$\mathbf{x} = \mathbf{P_A x} + (\mathbf{I} - \mathbf{P_A})\mathbf{x} = \mathbf{P_A x} + \mathbf{A Q_A A x} = \mathbf{P_A x} + \mathbf{A Q_A b}, \tag{5.5}$$

$$\mathbf{x} = \widetilde{\mathbf{P}}_\mathbf{A}\mathbf{x} + (\mathbf{I} - \widetilde{\mathbf{P}}_\mathbf{A})\mathbf{x} = \widetilde{\mathbf{P}}_\mathbf{A}\mathbf{x} + \mathbf{Q_A A}^2\mathbf{x} = \widetilde{\mathbf{P}}_\mathbf{A}\mathbf{x} + \mathbf{Q_A A b}. \tag{5.6}$$

Using (5.6), the system $\mathbf{Ax} = \mathbf{b}$ becomes $\mathbf{A}(\widetilde{\mathbf{P}}_\mathbf{A}\mathbf{x} + \mathbf{Q_A A b}) = \mathbf{b}$. With the definition of $\mathbf{P_A}$ and $\mathbf{A}\widetilde{\mathbf{P}}_\mathbf{A} = \mathbf{P_A A}$ (cf. Lemma 2.1) we see that this is equivalent to

$$\mathbf{P_A A x} = \mathbf{P_A b}.$$

We now substitute for $\mathbf{x}$ from (5.5) and obtain $\mathbf{P_A A}(\mathbf{P_A x} + \mathbf{A Q_A b}) = \mathbf{P_A b}$ which is equivalent to

$$\mathbf{P_A A P_A x} = \mathbf{P_A}\widetilde{\mathbf{P}}_\mathbf{A}^{\mathsf{H}}\mathbf{b}. \tag{5.7}$$

We can show the following result for the MinRes method applied to this symmetric system.

Theorem 5.1. *For each initial guess $\mathbf{x}_0 \in \mathbb{C}^N$ the* MinRes *method applied to the system (5.7) gives (in exact arithmetic) a well defined iterate $\overline{\mathbf{x}}_n$ at each step $n \geq 1$ until it terminates with a solution. Moreover, the sequence of iterates*

$$\mathbf{x}_n := \widetilde{\mathbf{P}}_\mathbf{A}\left(\mathbf{P_A}\overline{\mathbf{x}}_n + \mathbf{A Q_A b}\right) + \mathbf{Q_A A b} \tag{5.8}$$

is well defined. It terminates (in exact arithmetic) with the exact solution $\mathbf{x}$ of the original linear system $\mathbf{Ax} = \mathbf{b}$ and its residuals are given by $\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n = \mathbf{P_A}\widetilde{\mathbf{P}}_\mathbf{A}^{\mathsf{H}}\mathbf{b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n$.

Proof. The first part follows from the fact that the system (5.7) is a consistent system with a hermitian matrix $\mathbf{P_A A P_A}$, so that we can apply Theorem 4.1. It remains to show the second part. The n-th residual of the original system $\mathbf{Ax} = \mathbf{b}$ is given by

$$\begin{aligned}
\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{x}_n &= \mathbf{b} - \mathbf{A}\left(\widetilde{\mathbf{P}}_\mathbf{A}\left(\mathbf{P_A}\overline{\mathbf{x}}_n + \mathbf{A Q_A b}\right) + \mathbf{Q_A A b}\right) \\
&= \mathbf{b} - \mathbf{A}\widetilde{\mathbf{P}}_\mathbf{A}\left(\mathbf{P_A}\overline{\mathbf{x}}_n + \mathbf{A Q_A b}\right) - \mathbf{A Q_A A b} \\
&= \left(\mathbf{I} - \mathbf{A Q_A A}\right)\mathbf{b} - \mathbf{P_A A}\left(\mathbf{P_A}\overline{\mathbf{x}}_n + \mathbf{A Q_A b}\right) \\
&= \mathbf{P_A b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n - \mathbf{P_A A}^2\mathbf{Q_A b} \\
&= \mathbf{P_A}\left(\mathbf{I} - \mathbf{A}^2\mathbf{Q_A}\right)\mathbf{b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n \\
&= \mathbf{P_A}\widetilde{\mathbf{P}}_\mathbf{A}^{\mathsf{H}}\mathbf{b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n.
\end{aligned}$$

We see that $\mathbf{r}_n$ is equal to the nth MinRes residual for the system (5.7). In particular, this implies that the exact solution of (1.1) is given by (5.8) once a solution $\overline{\mathbf{x}}_n$ of (5.7) is determined by MinRes. ∎

The following theorem shows that a modification of the initial guess suffices to make the RMinRes method mathematically equivalent to MinRes applied to the system (5.7).

Theorem 5.2. *We consider the following two approaches:*

1. RMinRes *applied to* $\mathbf{Ax} = \mathbf{b}$ *with the initial guess* $\widetilde{\mathbf{x}}_0 := \mathbf{P_A x}_0 + \mathbf{AQ_A b}$ *and resulting iterates* $\mathbf{x}_n$ *and residuals* $\mathbf{r}_n = \mathbf{b} - \mathbf{Ax}_n$.
2. MinRes *applied to* (5.7) *with initial guess* $\mathbf{x}_0$ *and resulting iterates* $\overline{\mathbf{x}}_n$ *and residuals* $\overline{\mathbf{r}}_n := \mathbf{P_A}\widetilde{\mathbf{P}}_{\mathbf{A}}^{\mathsf{H}}\mathbf{b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n$.

Both approaches are equivalent in the sense that $\mathbf{x}_n = \widetilde{\mathbf{P}}_{\mathbf{A}}(\mathbf{P_A}\overline{\mathbf{x}}_n + \mathbf{AQ_A b}) + \mathbf{Q_A Ab}$ *and* $\mathbf{r}_n = \overline{\mathbf{r}}_n$.

Proof. Let us start with the MinRes method applied to (5.7), which constructs iterates $\overline{\mathbf{x}}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n$, where $\mathbf{V}_n \in \mathbb{C}^{N\times n}$ is of full rank n such that $\mathsf{Im}\,(\mathbf{V}_n) = \mathcal{K}_n(\mathbf{P_A A P_A}, \mathbf{P}\widetilde{\mathbf{P}}^{\mathsf{H}}\mathbf{r}_0)$. Then $\mathbf{P_A V}_n = \mathbf{V}_n$ and the corrected iterates are

$$\begin{aligned}\mathbf{x}_n &= \widetilde{\mathbf{P}}_{\mathbf{A}}(\mathbf{P_A}(\mathbf{x}_0 + \mathbf{V}_n\mathbf{y}_n) + \mathbf{AQ_A b}) + \mathbf{Q_A Ab} = \widetilde{\mathbf{P}}_{\mathbf{A}}(\widetilde{\mathbf{x}}_0 + \mathbf{V}_n\mathbf{y}_n) + \mathbf{Q_A Ab}\\ &= \widetilde{\mathbf{P}}_{\mathbf{A}}\widetilde{\mathbf{x}}_n + \mathbf{Q_A Ab},\end{aligned} \tag{5.9}$$

with $\widetilde{\mathbf{x}}_n := \widetilde{\mathbf{x}}_0 + \mathbf{V}_n\mathbf{y}_n$. For $n > 0$ the n-th residual of $\overline{\mathbf{x}}_n$ with respect to the system (5.7) is

$$\begin{aligned}\overline{\mathbf{r}}_n &= \mathbf{P_A}\widetilde{\mathbf{P}}_{\mathbf{A}}^{\mathsf{H}}\mathbf{b} - \mathbf{P_A A P_A}\overline{\mathbf{x}}_n = \mathbf{P_A}(\widetilde{\mathbf{P}}_{\mathbf{A}}^{\mathsf{H}}\mathbf{b} - \mathbf{AP_A x}_0 - \mathbf{AV}_n\mathbf{y}_n)\\ &= \mathbf{P_A}(\mathbf{b} - \mathbf{A}(\mathbf{P_A x}_0 + \mathbf{AQ_A b} + \mathbf{V}_n\mathbf{y}_n)) = \mathbf{P_A b} - \mathbf{P_A A}\widetilde{\mathbf{x}}_n =: \widetilde{\mathbf{r}}_n.\end{aligned}$$

This is the residual of $\widetilde{\mathbf{x}}_n$ with respect to the system (5.4). We also have

$$\widetilde{\mathbf{r}}_0 = \mathbf{P_A b} - \mathbf{P_A A}\widetilde{\mathbf{x}}_0 = \mathbf{P_A}\widetilde{\mathbf{P}}_{\mathbf{A}}^{\mathsf{H}}\mathbf{b} - \mathbf{P_A AP_A x}_0 = \overline{\mathbf{r}}_0,$$

and thus the starting vectors of the Krylov subspace for both methods are equal. Because of (5.2) also the Krylov subspaces are equal. From the definition of the Krylov subspaces we immediately obtain

$$\overline{\mathbf{r}}_n \perp \mathbf{P_A AP_A}\mathcal{K}_n(\mathbf{P_A AP_A}, \overline{\mathbf{r}}_0) \quad\Longleftrightarrow\quad \widetilde{\mathbf{r}}_n \perp \mathbf{P_A A}\mathcal{K}_n(\mathbf{P_A A}, \widetilde{\mathbf{r}}_0).$$

We can now see that the iterates $\widetilde{\mathbf{x}}_n$ are the iterates of MinRes applied to (5.4) with initial guess $\widetilde{\mathbf{x}}_0$. Along with the correction (5.9) this was shown to be equivalent to RMinRes applied to $\mathbf{Ax} = \mathbf{b}$ with initial guess $\widetilde{\mathbf{x}}_0$ (cf. Section 5.1). ∎

This means that (in exact arithmetic) breakdowns in RMinRes can be prevented by choosing the adapted initial guess $\widetilde{\mathbf{x}}_0$ defined in Theorem 5.2.

6. Numerical experiments. In this section, we will show the numerical behaviour of selected Krylov subspace methods discussed above. Detailed numerical experiments with the deflated CG method (cf. Section 3) and equivalent approaches have been presented in [22]. Here, we will focus on the RMinRes method and the deflated MinRes method (cf. Sections 5.1 and 5.2). Both methods are implemented in MATLAB with three-term Lanczos recurrences and Givens rotations for solving the least squares problem. All residuals have been computed explicitly in each iteration.

Example 6.1. In this example we use a matrix $\mathbf{A} = \mathbf{W}^{\mathsf{H}}\mathbf{DW} \in \mathbb{R}^{2m\times 2m}$, $m = 50$, where $\mathbf{D} = \mathrm{diag}(\lambda_1, \ldots, \lambda_{2m})$ with $\lambda_j = \sqrt{j}$, $\lambda_{m+j} = -\sqrt{j}$ for $j = 1, \ldots, m$ and $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_{2m}]$ is a randomly generated orthogonal matrix. We consider a deflation matrix $\mathbf{U} = [u_1, \ldots, u_k]$ whose columns are pairwise orthogonal eigenvectors of $\mathbf{A}$, i.e. $\mathbf{AU} = \mathbf{UD_U}$ and $\mathbf{U}^{\mathsf{H}}\mathbf{U} = \mathbf{I}_k$ with a diagonal matrix $\mathbf{D_U} = \mathrm{diag}(\lambda_{j_1}, \ldots, \lambda_{j_k})$ for $0 < j_1 < \cdots < j_k < 2m$. This means that $\mathcal{U} = \mathsf{Im}\,(\mathbf{U})$ is an exact $\mathbf{A}$-invariant subspace. Then a straightforward computation reveals that $\mathbf{P_A} = \widetilde{\mathbf{P}}_{\mathbf{A}} = \mathbf{I} - \mathbf{UU}^{\mathsf{H}}$, which is obviously hermitian, and

$$\mathbf{P_A AP_A} = \mathbf{P_A A}\widetilde{\mathbf{P}}_{\mathbf{A}} = \mathbf{P}_{\mathbf{A}}^2\mathbf{A} = \mathbf{P_A A}, \quad \mathbf{P_A}\widetilde{\mathbf{P}}_{\mathbf{A}}^{\mathsf{H}} = \mathbf{P}_{\mathbf{A}}^2 = \mathbf{P_A}.$$

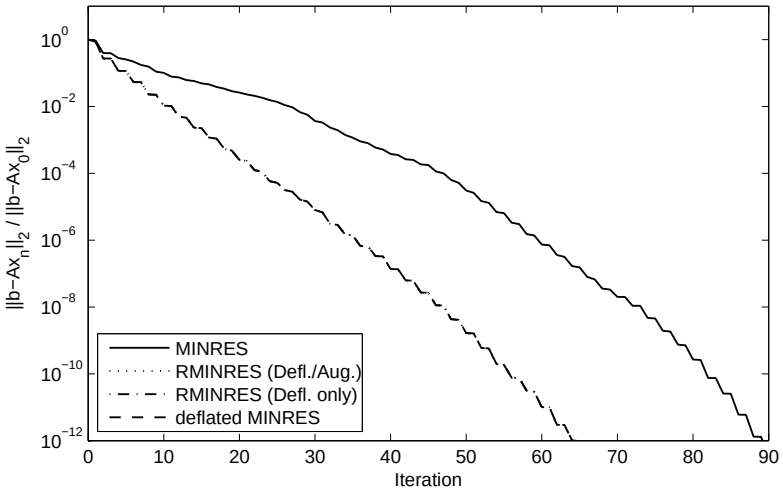


FIG. 6.1. *Convergence history for Example 6.1.*

By comparing the correction steps of RMINRES and deflated MINRES (cf. Sections 5.1 and 5.2) and using $\mathbf{P_A A Q_A} = \mathbf{0}$, we can see that both methods are mathematically equivalent if $\mathcal{U}$ is an exact invariant subspace.

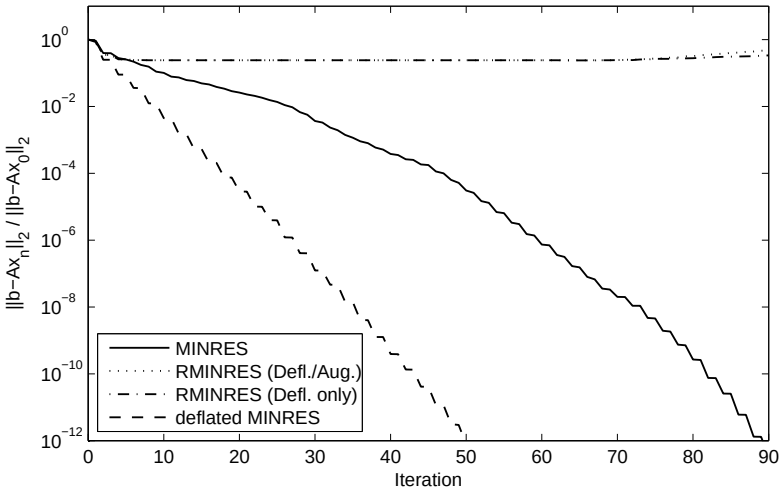
We solve the system $\mathbf{Ax} = \mathbf{b}$ with a random right-hand side $\mathbf{b}$ and the initial guess $\mathbf{x}_0 = \mathbf{0}$. In Figure 6.1 we show the relative residual norms of the solvers

- MINRES (solid line),
- RMINRES with explicit augmentation and deflation (dotted line) according to Wang et al. [23]; cf. (5.3),
- RMINRES with deflation only (dash-dotted line), i.e., the residual norms of MINRES applied to the system $\mathbf{P_A Ax} = \mathbf{P_A b}$; cf. (5.4),
- deflated MINRES (dashed line), i.e., the residual norms of MINRES applied to the system $\mathbf{P_A A P_A x} = \mathbf{P_A}\widetilde{\mathbf{P}}_\mathbf{A}^\mathsf{H}\mathbf{b}$; cf. Section 5.2.

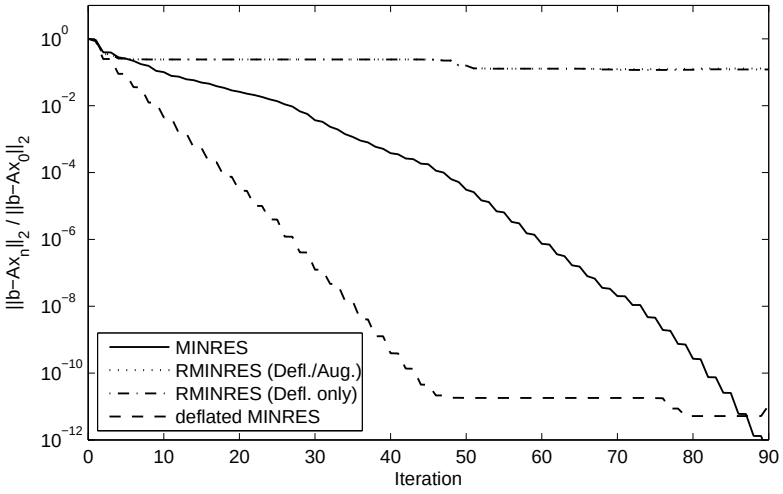
For the last three methods we used the matrix $\mathbf{U} = [\mathbf{w}_1, \ldots, \mathbf{w}_5, \mathbf{w}_{51}, \ldots, \mathbf{w}_{55}]$ which contains the eigenvectors associated with the 10 eigenvalues of $\mathbf{A}$ of smallest absolute value. Thus the deflation space $\mathcal{U}$ has dimension 10 and is an exact $\mathbf{A}$-invariant subspace. The numerical experiment illustrates our theoretical result that the two implementations of RMINRES and the deflated MINRES method are mathematically equivalent. Note that all three convergence curves coincide in Figure 6.1.

EXAMPLE 6.2. In this example we investigate breakdowns and near-breakdowns of the RMINRES method numerically. We use the same matrix $\mathbf{A}$ as in Example 6.1 and we construct a subspace $\mathcal{U}$ for which $\mathcal{U} \cap (\mathbf{A}\mathcal{U})^\perp \neq \{\mathbf{0}\}$. Thus, the condition that guarantees a breakdown-free RMINRES computation is violated; cf. Section 5.1.

To construct the subspace $\mathcal{U}$ we choose an integer k, $0 < k < m$, and we define $\mathbf{W}_1 = [\mathbf{w}_{i_1}, \ldots, \mathbf{w}_{i_k}]$ and $\mathbf{W}_2 = [\mathbf{w}_{m+i_1}, \ldots, \mathbf{w}_{m+i_k}]$ for indices $0 < i_1 < \cdots < i_k < m$. With $\mathbf{D_U} = \mathrm{diag}(\lambda_{i_1}, \cdots, \lambda_{i_k})$ we obtain $\mathbf{AW}_1 = \mathbf{W}_1\mathbf{D_U}$ and $\mathbf{AW}_2 = -\mathbf{W}_2\mathbf{D_U}$ because of the symmetry of the spectrum of $\mathbf{A}$. We now choose the deflation and augmentation matrix as $\mathbf{U} = \mathbf{W}_1 + \mathbf{W}_2$. Applying $\mathbf{A}$ yields $\mathbf{AU} = (\mathbf{W}_1 - \mathbf{W}_2)\mathbf{D_U}$ and using the fact that $\mathbf{W}$ is unitary shows that $\mathbf{U}^\mathsf{H}\mathbf{AU} = \mathbf{0}$, or equivalently $\mathcal{U} \subset (\mathbf{A}\mathcal{U})^\perp$. The proof of Theorem 4.1 gives us a way to construct an initial guess which leads to an immediate breakdown of RMINRES. For an arbitrary $\mathbf{0} \neq \mathbf{u} \in \mathcal{U}$ we choose $\mathbf{x}_0 = \mathbf{A}^{-1}(\mathbf{b} - \mathbf{u})$. Because of $\mathcal{U} \perp \mathbf{A}\mathcal{U}$ we have $\mathbf{P_A u} = \mathbf{u}$ and the initial residual



(a) Unperturbed deflation space $\mathbf{U}^{(1)}$



(b) Perturbed deflation space $\mathbf{U}^{(2)} = \mathbf{U}^{(1)} + \mathbf{E}$

FIG. 6.2. *Convergence history for Example 6.2.*

of RMINRES is $\mathbf{r}_0 = \mathbf{P_A b} - \mathbf{P_A A x}_0 = \mathbf{u}$. The breakdown then occurs in the first iteration because $\mathbf{P_A A r}_0 = \mathbf{P_A A u} = \mathbf{0}$ since $\mathbf{Au} \in \mathbf{A}\mathcal{U} = \mathsf{ker}\,(\mathbf{P_A})$.

For these constructed initial guesses the RMINRES method indeed breaks down immediately in numerical experiments, whereas the deflated MINRES method finds the solution after one step. However, of greater interest are situations with perturbed initial guesses. Interestingly also random initial guesses lead to a breakdown of RMINRES after a few steps.

In Figure 6.2 we again show the relative residual norms of the solvers listed above applied to exactly the same $\mathbf{A}$, $\mathbf{b}$ and $\mathbf{x}_0$ as in the previous example. For Figure 6.2(a) we used the matrix $\mathbf{U}^{(1)} = [\mathbf{w}_1 + \mathbf{w}_{51}, \ldots, \mathbf{w}_{10} + \mathbf{w}_{60}]$ whereas Figure 6.2(b) shows the results for a perturbed matrix $\mathbf{U}^{(2)} = \mathbf{U}^{(1)} + \mathbf{E}$ with a random $\mathbf{E} \in \mathbb{C}^{100\times 10}$ and $||\mathbf{E}||_2 = 10^{-10}$. Then both deflation spaces again have dimension 10.

Note that both RMinRes implementations suffer from a breakdown after a few steps with both matrices $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$. With the unperturbed matrix $\mathbf{U}^{(1)}$ the deflated MinRes method converges to the solution with relative residual smaller than 10^{-12}, while in the case of the perturbed matrix $\mathbf{U}^{(2)}$ the method stagnates with a relative residual of order 10^{-11}. This stagnation of deflated MinRes seems to be related to an unfavorable spectrum of $\mathbf{P_A A P_A}$ for these specifically constructed and perturbed matrices like $\mathbf{U}^{(2)}$. Perturbing the matrix $\mathbf{U}$ from Example 6.1 whose columns are exact eigenvectors of $\mathbf{A}$ does not cause stagnation. This behaviour is still subject to further research.

7. Conclusions. In this paper we first analyzed theoretically the link between deflated and augmented Krylov subspace methods whose residuals satisfy a (Petrov-) Galerkin condition. For the CG method and GMRes/MinRes methods we have seen that augmentation can be achieved without explicitly enhancing the Krylov subspace, but instead projecting the residuals appropriately and using a correction for the approximate solutions.

The projections which arise from the augmentation can also used to obtain a deflated system. We have seen that a left-multiplication of the original system with the corresponding projection yields a deflated system for which the CG method and GMRes/MinRes methods implicitly achieve augmentation. We proved that for nonsingular hermitian matrices the MinRes method for the deflated system is equivalent to the RMinRes method introduced in [23]. While CG never breaks down, GMRes, MinRes and thus RMinRes may suffer from breakdowns when used with the deflated systems. We stated necessary and sufficient conditions to characterize breakdowns of these minimal residual methods. For hermitian matrices, we introduced the deflated MinRes method which also uses a hermitian deflated matrix and proved that it cannot break down.

In numerical experiments we compared the MinRes, RMinRes and deflated MinRes methods. With exact invariant subspaces as deflation spaces the iterates of RMinRes and deflated MinRes coincide as expected. Using a contrived deflation space led to a breakdown of RMinRes for random initial guesses and even with small perturbations of the deflation space. In this particular example, the deflated MinRes method still converged when no perturbations have been added but suffered from stagnation otherwise, which is under further investigation.

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