SIAM J. MATRIX ANAL. APPL.
Vol. 35, No. 4, pp. 1444–1466

DEFLATED AND AUGMENTED KRYLOV SUBSPACE METHODS: A FRAMEWORK FOR DEFLATED BICG AND RELATED SOLVERS*

MARTIN H. GUTKNECHT†

Abstract. We present an extension of the framework of Gaul et al. [*SIAM J. Matrix Anal. Appl.*, 34 (2013), pp. 495–518] for deflated and augmented Krylov subspace methods satisfying a Galerkin condition to more general Petrov–Galerkin conditions. The main goal is to apply the framework to the biconjugate gradient method (BiCG) and some of its generalizations, including BiCGStab and IDR(s). For such applications the assumptions of Gaul et al. were too restrictive. Our abstract approach does not depend on particular recurrences and thus simplifies the derivation of theoretical results. It easily leads to a variety of realizations by specific algorithms. We do not go into algorithmic details, but we show that for every method there are two different approaches for extending it by augmentation and deflation: one that explicitly takes care of the augmentation space in every step, and one that applies the appropriate Krylov subspace method to a projected problem but requires a correction step at the end. The latter approach typically generates nested sequences of Krylov subspaces for a singular operator that is associated with the projected problem. The deflated BiCG method requires two such sequences, but it also allows us to solve two dual linear systems at the price of one, a property that no longer holds for the closely related deflated biconjugate residual method (BiCR). Deflated Lanczos-type product methods fit in our new framework too. The question of how to extract the augmentation and deflation subspaces is not addressed here.

Key words. Krylov subspace methods, augmentation, deflation, Krylov subspace recycling, BiCG, biconjugate gradient method, BiCR, biconjugate residual method, BiCGStab, block BiCG, ML(s)BiCG, ML(s)BiCGStab, IDR(s)

AMS subject classifications. 65F10, 65F08

DOI. 10.1137/130923087

1. Introduction.

We consider the solution of a given linear algebraic system $\mathbf{A}\mathbf{x} = \mathbf{b}$, with $\mathbf{A} \in \mathbb{C}^{N\times N}$ nonsingular and $\mathbf{b} \in \mathbb{C}^N$, with a Krylov subspace method that is based on a Petrov–Galerkin condition. Such a method produces a sequence of approximate solutions $\mathbf{x}_n$ chosen from an affine solution search space[1] $\mathbf{x}_0 + \mathcal{S}_n$, such that their residuals $\mathbf{r}_n := \mathbf{b} - \mathbf{A}\mathbf{x}_n$, which lie in the corresponding affine residual search space $\mathbf{r}_0 + \mathbf{A}\mathcal{S}_n$, satisfy a Petrov–Galerkin condition:

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{S}_n\,, \qquad \mathbf{r}_n \in \mathbf{r}_0 + \mathbf{A}\mathcal{S}_n\,, \qquad \mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{S}}_n\,. \tag{1.1}$$

Here $\widetilde{\mathcal{S}}_n$ is a linear test space that is assumed to have the same dimension as $\mathcal{S}_n$, while $\mathbf{B} \in \mathbb{C}^{N\times N}$ is a nonsingular matrix, which we may think of as a possibly indefinite inner product matrix. The inclusion of such an optional $\mathbf{B}$ has been promoted by Young and Jea [63], Ashby, Manteuffel, and Saylor [8], and many others. In Gaul et al. [28][2] this was in particular used to cover the deflated conjugate gradient (CG) and deflated MinRes methods in the same framework. For the biconjugate gradient

*Received by the editors May 31, 2013; accepted for publication (in revised form) by M. E. Kilmer September 17, 2014; published electronically December 4, 2014.
http://www.siam.org/journals/simax/35-4/92308.html

†Seminar for Applied Mathematics, ETH Zurich, CH-8092 Zurich, Switzerland (mhg@math.ethz.ch). The author started his research while visiting the TU Berlin and was supported by the DFG Forschungszentrum MATHEON and the Mercator Visiting Professorship Program of the DFG.

[1]For simplicity we will sometimes refer to the subspace $\mathcal{S}_n$ as the (solution) search space.

[2]By the time the present article became ready for printing, Gaul's related Ph.D. thesis [26] had been made available.

method (BiCG) [20, 35] based on the non-Hermitian Lanczos process this generalization was introduced in [29, 30], but seen to be more restrictive: $\mathbf{A}$ and $\mathbf{B}$ must commute. Here, for deflated BiCG, we will encounter an additional restriction.

In many applications, deflation and augmentation techniques have been successfully applied to speed up the convergence of Krylov subspace methods. This is typically achieved by removing from the problem eigenvalues of $\mathbf{A}$ that are close to 0, a process called deflation. In the non-Hermitian case addressed here additional spectral properties may be important for the effectiveness of deflation. In any case, recall that we want to find $\mathbf{A}^{-1}\mathbf{b} = \mathbf{x}_0 + \mathbf{A}^{-1}\mathbf{r}_0$; so we need $\mathbf{A}^{-1}\mathbf{r}_0$. Assume the known columns of $\mathbf{U} \in \mathbb{C}^{N\times k}$ span an approximately invariant subspace $\mathcal{U}$ of $\mathbf{A}$, and let $\mathbf{Z} := \mathbf{AU}$, $\mathcal{Z} := \mathbf{A}\mathcal{U}$. Note that the images of the restriction $\mathbf{A}^{-1}\big|_{\mathcal{Z}}$ are trivial to compute: if $\mathbf{z} = \mathbf{Zc} \in \mathcal{Z}$, then $\mathbf{A}^{-1}\mathbf{z} = \mathbf{Uc}$. This still holds if $\mathcal{U}$ is not an invariant subspace. Assume further that we know another k-dimensional subspace $\widetilde{\mathcal{U}}$ such that $\mathbb{C}^N$ splits up according to $\mathcal{Z} \oplus (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp} = \mathbb{C}^N$, where this direct sum need not be an orthogonal decomposition. (Of course, it is if we choose $\widetilde{\mathcal{U}} := \mathbf{B}^{-\mathsf{H}}\mathcal{Z}$.) We can split up $\mathbf{r}_0$ accordingly: by applying the projection $\mathbf{P}$ with null space $\mathcal{N}(\mathbf{P}) = \mathcal{Z}$ and range $\mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ we can construct $\widehat{\mathbf{r}}_0 := \mathbf{P}\mathbf{r}_0 \in (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ such that

$$\mathbf{r}_0 = \underbrace{\mathbf{r}_0 - \widehat{\mathbf{r}}_0}_{\in \mathcal{N}(\mathbf{P}) = \mathcal{Z}} + \underbrace{\widehat{\mathbf{r}}_0}_{\in \mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}}. \tag{1.2}$$

Here, $\mathbf{A}^{-1}(\mathbf{r}_0 - \widehat{\mathbf{r}}_0)$ is trivial to compute. So, it remains to compute $\mathbf{A}^{-1}\widehat{\mathbf{r}}_0$. This problem can be addressed with a Krylov solver. In the ideal situation where $\mathcal{U}$ and, hence, $\mathcal{Z}$ are exactly invariant and represent all the eigenvalues close to 0, $\widehat{\mathbf{r}}_0$ will not have an eigenvector component associated with a small eigenvalue if $\widetilde{\mathcal{U}}$ has been chosen the right way, namely, such that $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ is also $\mathbf{A}$-invariant and represents the other eigenvalues of $\mathbf{A}$; see [32]. Then, in theory, we could just replace $\mathbf{A}$ by a singular, *"deflated"* matrix $\widehat{\mathbf{A}}$ (defined later) and apply the solver with the initial approximation $\widehat{\mathbf{x}}_0 := \mathbf{0}$ to $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ (instead of $\mathbf{A}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$) with the solution restricted to $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$. In this situation, for both $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ and $\mathbf{A}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$, the solver will just act on $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$. In a more realistic situation, neither $\mathcal{Z}$ nor $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ will be exactly $\mathbf{A}$-invariant. A fortiori it is important to solve the so restricted system $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$, which is typically much better conditioned than $\mathbf{A}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$. In the nonrestricted latter system any components of $\widehat{\mathbf{r}}_0$ that belong to small eigenvalues of $\mathbf{A}$ might get dramatically amplified. Using $\widehat{\mathbf{A}}$ restricted to $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ instead of $\mathbf{A}$ will make the Krylov solver behave more stably with respect to such bad components of $\widehat{\mathbf{r}}_0$ and also with respect to roundoff.

The Krylov subspaces $\widehat{\mathcal{K}}_n$ generated by $\widehat{\mathbf{A}}$ from the initial projected residual $\widehat{\mathbf{r}}_0$ will be contained in $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$. As suggested by (1.2), to represent (or at least approximate) $\mathbf{A}^{-1}\mathbf{r}_0$ we could use approximations $\widehat{\mathbf{x}}_n$ of $\mathbf{A}^{-1}\widehat{\mathbf{r}}_0$ shifted by $\mathbf{A}^{-1}(\mathbf{r}_0 - \widehat{\mathbf{r}}_0) \in \mathcal{U}$. Hence, we *"augment"* $\widehat{\mathcal{K}}_n$ by $\mathcal{U}$. So, this approach involves both *deflation* of approximate eigenvalues and *augmentation* of the Krylov subspaces $\widehat{\mathcal{K}}_n$. However, for simplicity we will often just refer to methods as deflated (as most other authors do) when we actually mean "deflated and augmented" methods. In fact, deflation makes no sense without augmentation here, though methods do exist that apply augmentation of the search space but no deflation of the matrix. One such method due to Saad fits into the framework of flexible GMRes [46]. We also need to mention that some authors use the seemingly more general terminology "Krylov subspace recycling methods" for deflated and augmented Krylov subspace methods [5, 6, 34, 44]. There are various

options for choosing $\widetilde{\mathcal{U}}$ and $\widehat{\mathbf{A}}$. For example, in the CG method for Hermitian positive definite systems the goal will be to maintain the property that the error vectors have minimum energy norm (or, equivalently, that $\mathbf{r}_n$ is orthogonal to the solution search space). This has been achieved by the algorithms of Nicolaides [42] and Dostál [13], and more than ten years later by those of Erhel and Guyomarc'h [16] and Saad et al. [47]. Likewise, for the BiCG method the goal will be to maintain the property that the residuals are orthogonal to the search space for the solution of a dual problem. This will be achieved here.

Similarly, one can aim for a method where the 2-norm of the residuals is minimal, as in the recycling MinRes method of Wang, de Sturler, and Paulino [57] or in a corresponding deflated GMRes method, of which several versions have been proposed [11, 12, 28, 32, 37, 38]. Even if we assume that the procedure for choosing the approximately invariant subspace is fixed, there are various options for defining the restricted matrix $\widehat{\mathbf{A}}$, and we will concentrate here on a particular way to do that.

The deflated versions of CG and MinRes mentioned above, as well as a deflated GMRes method, have been characterized in the framework of [28]. In the present paper we extend the framework of [28], which assumed a Galerkin condition to hold for the residuals, to the more general Petrov–Galerkin condition (1.1), which allows for two different spaces $\mathcal{S}_n$ and $\widetilde{\mathcal{S}}_n$. This generalization is significant, since it allows one to study and characterize methods based on the non-Hermitian Lanczos process such as the BiCG method and some of its generalizations, including BiCGStab [55] and IDR(s) [53]. For an introduction to BiCG and related algorithms published up to 1996, see [30]; for an introduction to IDR(s), see [53] or [31]. Compared to other Krylov subspace solvers, BiCG has the disadvantage of requiring two matrix-vector products (matvecs) per iteration, one with $\mathbf{A}$ and one with $\mathbf{A}^{\mathsf{H}}$. On the other hand, at essentially the cost of solving one system, $\mathbf{A}\mathbf{x} = \mathbf{b}$, one can additionally solve a second, dual system, $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$. In section 4 we will explore if and how this benefit can be preserved under deflation and augmentation.

We need to admit that the above-described recipe for a deflation and augmentation method based on the splitting (1.2) and the iterative solution of $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ does not exactly reflect the methods cited above and those proposed here later. In fact, it would yield residuals $\mathbf{r}_n := \mathbf{r}_0 - (\mathbf{r}_0 - \widehat{\mathbf{r}}_0) - \widehat{\mathbf{A}}\widehat{\mathbf{x}}_n = \widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}\widehat{\mathbf{x}}_n =: \widehat{\mathbf{r}}_n$ whose component in $\mathcal{Z}$ does not depend on n. In contrast, the component in $\mathcal{Z}$ of our residuals $\mathbf{r}_n$ will depend on n since they are forced to fulfill a Petrov–Galerkin condition that depends on n; see (2.3) below.

We also need to mention that there are other ways to recycle Krylov subspace information that do not fit into our new framework. For example, it has been suggested to augment the Krylov subspace basis, but to project the residuals not in every step but only occasionally [37, 38], or even just for modifying the initial approximation $\mathbf{x}_0$ as in InitCG by Erhel and Guyomarc'h [16]. Another approach is to apply a nonsingular preconditioner based on spectral information instead of the singular preconditioners used for deflation. For partial overviews of augmentation and deflation methods, see, e.g., [11, 14, 28, 32, 38, 44, 48].

The framework of [32] differs from the one here in that it promotes Krylov subspace methods with "true" deflation in the sense that $\mathbf{A}\big|_{\mathcal{Z}} = \mathbf{O}\big|_{\mathcal{Z}}$ and $\mathbf{A}\big|_{\widetilde{\mathcal{Z}}^\perp} = \widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^\perp}$ if $\mathcal{Z}$ is exactly $\mathbf{A}$-invariant and $\widetilde{\mathcal{Z}}$ is the corresponding $\mathbf{A}^{\mathsf{H}}$-invariant subspace. Sometimes this property will also be achieved here. Another difference is that [32] concentrates on coordinate-space-based methods, that is, methods like GMRes, where bases of the Krylov subspaces are constructed first and the linear system is expressed

in terms of the coordinates with respect to these bases. The solution of the so transplanted deflated and augmented problem is then described for a number of such methods.

Outline. In section 2 we define and characterize a family of augmented and deflated Krylov subspace methods for non-Hermitian problems. The characteristic properties of particular methods are treated in sections 3–6. As mentioned above, we notably cover a number of (non-Hermitian) Lanczos-type methods, including BiCG, the biconjugate residual method (BiCR), and some related methods such as BiCGStab, ML(s)BiCG, ML(s)BiCGStab, and IDR(s). Finally, section 7 is devoted to spectral result for the deflated operator $\widehat{\mathbf{A}}$.

2. A generalized framework for deflated and augmented Krylov subspace methods. In this section we extend the general framework for deflation and augmentation described in [28] in order to include Krylov subspace methods for non-Hermitian matrices that are based on a Petrov–Galerkin condition. We start from the basic setting of (1.1), where we now assume that both the search space $\mathcal{S}_n$ and the test space $\widetilde{\mathcal{S}}_n$ are augmented:

$$\mathcal{S}_n = \widehat{\mathcal{K}}_n + \mathcal{U}\,, \qquad \widetilde{\mathcal{S}}_n = \widehat{\mathcal{L}}_n + \widetilde{\mathcal{U}}\,. \tag{2.1}$$

Here, $\mathcal{U}$ and $\widetilde{\mathcal{U}}$ are called the augmentation spaces. Their suitable choice has been quickly addressed in the introduction; many suggestions for selected types of problems can be found in the literature; see, e.g., [1, 5, 6, 12, 34, 37, 38, 44, 57]. Theoretical results on invariant subspaces will be given in section 7.

For the moment we leave it open how the subspaces $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ are defined. In the most typical situation they are Krylov subspaces or block Krylov subspaces, but we will also encounter situations where their structure is more complicated. We assume that both have the same dimension n and that the columns of $\mathbf{V}_n$ and $\widetilde{\mathbf{V}}_n \in \mathbb{C}^{N\times n}$ form bases of $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$, respectively. Similarly, the columns of $\mathbf{U}$ and $\widetilde{\mathbf{U}}$ form bases of the augmentation spaces $\mathcal{U}$ and $\widetilde{\mathcal{U}}$. Of course, $\mathcal{U}$ and $\widetilde{\mathcal{U}}$ may be redefined when an algorithm is restarted, but we will not account for that in our notation. Let us further define

$$\mathbf{Z} := \mathbf{A}\mathbf{U}\,, \qquad \mathcal{Z} := \mathbf{A}\mathcal{U}$$

and, for later use,

$$\widetilde{\mathbf{Z}} := \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{U}}\,, \qquad \widetilde{\mathcal{Z}} := \mathbf{A}^{\mathsf{H}}\widetilde{\mathcal{U}}\,.$$

Then $\mathbf{x}_n$ and $\mathbf{r}_n$ can be represented as[3]

$$\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{c}_n + \mathbf{U}\mathbf{u}_n\,, \tag{2.2}$$

$$\mathbf{r}_n = \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n - \mathbf{Z}\mathbf{u}_n\,, \tag{2.3}$$

with some coordinate vectors $\mathbf{c}_n \in \mathbb{C}^n$ and $\mathbf{u}_n \in \mathbb{C}^k$.

With the choice (2.1) the Petrov–Galerkin condition in (1.1) implies that

$$\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\,\widehat{\mathcal{L}}_n \quad \text{and} \quad \mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\,\widetilde{\mathcal{U}}\,. \tag{2.4}$$

[3] Of course, if we do not have direct sums in (2.1), the representation may be nonunique, which might cause a problem.

On the left, we have a condition involving a growing test space, as is typical for Krylov subspace solvers based on a Galerkin or Petrov–Galerkin condition, while on the right we have an orthogonality condition that compensates for the deflation and will allow us to reduce the search and test spaces. Let us first concentrate on the second condition, which turns into the equality

$$\mathbf{0} = \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{r}_n = \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n - \mathbf{A}\mathbf{U}\mathbf{u}_n\right) = \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right) - \mathbf{E}\mathbf{u}_n\,,$$

where $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\mathbf{U}$. In the following, we will assume that $\mathbf{E}$ is nonsingular, so that we obtain for $\mathbf{u}_n$ in terms of $\mathbf{c}_n$ the explicit formula

$$\mathbf{u}_n = \mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right). \tag{2.5}$$

Using this and $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$ in (2.2) and (2.3) gives

$$\begin{aligned}\mathbf{x}_n &= \mathbf{x}_0 + \mathbf{V}_n\mathbf{c}_n + \mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right)\\ &= \left(\mathbf{I} - \mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\right)\left(\mathbf{x}_0 + \mathbf{V}_n\mathbf{c}_n\right) + \mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{b}, \qquad (2.6)\\ \mathbf{r}_n &= \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right)\\ &= \left(\mathbf{I} - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\right)\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right). \qquad (2.7)\end{aligned}$$

TABLE 1

Basic properties of the projections and other operators used in this paper. All these properties are easy to verify, and thus formal proofs are skipped for brevity. Note that $\mathbf{E}$ *and* $\widetilde{\mathbf{E}}$ *are* $k \times k$ *matrices, while all the other matrices have size* $N \times N$.

	Definition	Null space	Range	Further properties
$\mathbf{E}$	$\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\mathbf{U}$	$\{\mathbf{0}\}$	$\mathbb{C}^k$	assumed to be nonsingular
$\mathbf{M}$	$\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}$	$\widetilde{\mathcal{U}}^{\perp}$	$\mathcal{U}$	$\mathsf{rank}\,\mathbf{M} = k$
$\mathbf{P}$	$\mathbf{I} - \mathbf{A}\mathbf{M}\mathbf{B}$	$\mathcal{Z}$	$(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$\mathbf{P}^2 = \mathbf{P}$
$\mathbf{Q}$	$\mathbf{I} - \mathbf{M}\mathbf{B}\mathbf{A}$	$\mathcal{U}$	$(\mathbf{A}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$\mathbf{Q}^2 = \mathbf{Q}$
$\widehat{\mathbf{A}}$	$\mathbf{P}\mathbf{A}$	$\mathcal{U}$	$(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$\widehat{\mathbf{A}} = \mathbf{P}\mathbf{A} = \mathbf{A}\mathbf{Q} = \mathbf{P}\mathbf{A}\mathbf{Q}$
$\widehat{\mathbf{A}}^{\mathsf{H}}$	$\mathbf{Q}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}$	$\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$	$\mathcal{U}^{\perp}$	$\widehat{\mathbf{A}}^{\mathsf{H}} = \mathbf{Q}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}} = \mathbf{A}^{\mathsf{H}}\mathbf{P}^{\mathsf{H}} = \mathbf{Q}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}^{\mathsf{H}}$
$\widetilde{\mathbf{E}}$	$\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{U}}$	$\{\mathbf{0}\}$	$\mathbb{C}^k$	assumed to be nonsingular
$\widetilde{\mathbf{M}}$	$\widetilde{\mathbf{U}}\widetilde{\mathbf{E}}^{-1}\mathbf{U}^{\mathsf{H}}$	$\mathcal{U}^{\perp}$	$\widetilde{\mathcal{U}}$	$\mathsf{rank}\,\widetilde{\mathbf{M}} = k$
$\widetilde{\mathbf{P}}$	$\mathbf{I} - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{M}}\mathbf{B}^{\mathsf{H}}$	$\widetilde{\mathcal{Z}}$	$(\mathbf{B}\mathcal{U})^{\perp}$	$\widetilde{\mathbf{P}}^2 = \widetilde{\mathbf{P}}$
$\widetilde{\mathbf{Q}}$	$\mathbf{I} - \widetilde{\mathbf{M}}\mathbf{B}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}$	$\widetilde{\mathcal{U}}$	$(\mathbf{A}\mathbf{B}\mathcal{U})^{\perp}$	$\widetilde{\mathbf{Q}}^2 = \widetilde{\mathbf{Q}}$
$\widetilde{\mathbf{A}}$	$\widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}}$	$\widetilde{\mathcal{U}}$	$(\mathbf{B}\mathcal{U})^{\perp}$	$\widetilde{\mathbf{A}} = \widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}} = \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{Q}} = \widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{Q}}$
$\widetilde{\mathbf{A}}^{\mathsf{H}}$	$\widetilde{\mathbf{Q}}^{\mathsf{H}}\mathbf{A}$	$\mathbf{B}\mathcal{U}$	$\widetilde{\mathcal{U}}^{\perp}$	$\widetilde{\mathbf{A}} = \widetilde{\mathbf{Q}}^{\mathsf{H}}\mathbf{A} = \mathbf{A}\widetilde{\mathbf{P}}^{\mathsf{H}} = \widetilde{\mathbf{Q}}^{\mathsf{H}}\mathbf{A}\widetilde{\mathbf{P}}^{\mathsf{H}}$

After introducing

$$\mathbf{M} := \mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}, \qquad \mathbf{P} := \mathbf{I} - \mathbf{A}\mathbf{M}\mathbf{B}, \qquad \mathbf{Q} := \mathbf{I} - \mathbf{M}\mathbf{B}\mathbf{A}, \tag{2.8}$$

(2.6) and (2.7) take the form

$$\mathbf{x}_n = \mathbf{Q}\left(\mathbf{x}_0 + \mathbf{V}_n\mathbf{c}_n\right) + \mathbf{M}\mathbf{B}\mathbf{b}\,, \tag{2.9}$$

$$\mathbf{r}_n = \mathbf{P}\left(\mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{c}_n\right)\,, \tag{2.10}$$

exactly as in [28].[4] Note that $\mathbf{u}_n$ has been eliminated and no longer appears here. See Table 1 for some properties of the matrices $\mathbf{M}$, $\mathbf{P}$, and $\mathbf{Q}$. In particular, $\mathbf{P}$ and $\mathbf{Q}$ are projections, which, in general, are oblique.

[4] Take into account that our $\mathbf{B}$ corresponds to $\mathbf{B}^{\mathsf{H}}$ in [28]. Also note that $\mathbf{E}$, $\mathbf{M}$, $\mathbf{P}$, and $\mathbf{Q}$ depend on $\mathbf{B}$, a dependence that was made explicit in the notation of [28].

Imposing the first orthogonality condition of (2.4) will yield $\mathbf{c}_n$. To this end, let[5]

$$\widehat{\mathbf{x}}_n := \mathbf{x}_0 + \mathbf{V}_n\mathbf{c}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n\,, \qquad \widehat{\mathbf{r}}_n := \mathbf{P}(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_n)\,; \tag{2.11}$$

in particular, $\widehat{\mathbf{x}}_0 := \mathbf{x}_0$ and $\widehat{\mathbf{r}}_0 := \mathbf{P}\mathbf{r}_0 \perp \mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$. Then $\mathbf{x}_n = \mathbf{Q}\widehat{\mathbf{x}}_n + \mathbf{MBb}$, and by inserting (2.10) the first orthogonality condition becomes

$$\mathbf{r}_n = \mathbf{P}(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_n) = \widehat{\mathbf{r}}_n \perp \mathbf{B}^{\mathsf{H}}\widehat{\mathcal{L}}_n.$$

Thus we have shown the following theorem, which generalizes Theorem 3.2 in [28].

THEOREM 2.1. *Let* $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{N\times N}$ *and* $\mathbf{U}, \widetilde{\mathbf{U}} \in \mathbb{C}^{N\times k}$ *be such that* $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU}$ *is nonsingular, so that the matrices* $\mathbf{M}, \mathbf{P}, \mathbf{Q}$ *of* (2.8) *are well defined. Let* $\mathcal{U} := \mathcal{R}(\mathbf{U})$*, let* $\widetilde{\mathcal{U}} := \mathcal{R}(\widetilde{\mathbf{U}})$*, and, for some* $n \geq 1$*, let* $\widehat{\mathcal{K}}_n$ *and* $\widehat{\mathcal{L}}_n$ *be two subspaces of dimension* n*. Then the two pairs of conditions*

$$\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}\,, \qquad \mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}(\widehat{\mathcal{L}}_n + \widetilde{\mathcal{U}}) \tag{2.12}$$

and

$$\widehat{\mathbf{x}}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n\,, \qquad \widehat{\mathbf{r}}_n \perp \mathbf{B}^{\mathsf{H}}\widehat{\mathcal{L}}_n\,, \tag{2.13}$$

if determining $\mathbf{x}_n$ *and* $\widehat{\mathbf{x}}_n$ *uniquely, are equivalent in the sense that*

$$\mathbf{x}_n = \mathbf{Q}\widehat{\mathbf{x}}_n + \mathbf{MBb} \quad \textit{and} \quad \mathbf{r}_n = \widehat{\mathbf{r}}_n\,. \tag{2.14}$$

The rationale behind considering both (2.12) and (2.13) is that in an algorithm based on (2.12) we choose $\mathbf{x}_n$ from an augmented search space and enforce $\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}(\widehat{\mathcal{L}}_n + \widetilde{\mathcal{U}})$; in contrast, an algorithm based on (2.13) chooses $\widehat{\mathbf{x}}_n$ from a smaller space and fulfills $\widehat{\mathbf{r}}_n \perp \mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$ by construction, because $\widehat{\mathbf{r}}_n \in \mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$, and then needs only to enforce $\widehat{\mathbf{r}}_n \perp \mathbf{B}^{\mathsf{H}}\widehat{\mathcal{L}}_n$.

We can conclude that for each augmented and deflated iterative method characterized by the choices for $\mathbf{B}$, $\mathcal{U}$, $\widetilde{\mathcal{U}}$, $\widehat{\mathcal{K}}_n$, and $\widehat{\mathcal{L}}_n$ there are two equivalent approaches to realize the method—even before we come to the additional freedom of choosing the recurrences that yield the iterates and residuals fulfilling the given conditions (1.1) with the additive structure (2.1). The conditions (2.12) represent the *explicit deflation and augmentation approach*, where the augmentation space $\mathcal{U}$ is explicitly included in the search space. In the equivalent conditions (2.13) the explicit inclusion of $\mathcal{U}$ is replaced by a suitable projection of a restricted problem: we first construct iterates $\widehat{\mathbf{x}}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n$ without components in $\mathcal{U}$ such that the *projected residuals* $\widehat{\mathbf{r}}_n = \mathbf{P}(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_n)$ satisfy the simplified Petrov–Galerkin condition of (2.13); then we apply the affine correction (2.14). Interestingly, the projected residuals are equal to the original ones. We call this the *implicit deflation and augmentation approach*. Of course, in both approaches the restriction $\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$ is taken care of—either explicitly or by using the projection $\mathbf{P}$—but there is a fundamental difference between the two approaches that is apparent from the existence of the nontrivial relationship (2.14).

While the choice of $\mathbf{U}$ and $\widetilde{\mathbf{U}}$ is problem dependent and will not be addressed here, the most important options for $\mathbf{B}$, $\widehat{\mathcal{K}}_n$, and $\widehat{\mathcal{L}}_n$ will be discussed now and in the following sections. So far we have left it open how $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ are defined. Not every pair of subspaces will make sense. In the theorem we limit the choice by requesting

[5] What was $\widehat{\mathbf{x}}_n$ in section 1 is now called $\widehat{\mathbf{x}}_n - \mathbf{x}_0$.

that both $\mathbf{x}_n$ and $\widehat{\mathbf{x}}_n$ be uniquely determined by (2.12) and (2.13), respectively. By our derivation, every solution $\mathbf{x}_n$ of (2.12) yields a solution of (2.13), and due to the uniqueness assumption, the reverse holds too.

We are not really interested in utmost generality. The methods we aim at are all Krylov subspace methods or block Krylov subspace methods satisfying suitable Petrov–Galerkin conditions.

According to its definition, $\widehat{\mathbf{r}}_n$ is the residual of the approximate solution $\widehat{\mathbf{x}}_n$ of the projected or deflated linear system

$$\mathbf{PA}\widehat{\mathbf{x}} = \mathbf{Pb}\,. \tag{2.15}$$

Since $\widehat{\mathbf{x}}_n - \mathbf{x}_0 \in \widehat{\mathcal{K}}_n$, and since both sides of the system lie in $\mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$, we want to solve it by a Krylov subspace method that is fully restricted to $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$. Defining

$$\widehat{\mathbf{A}} := \mathbf{PA} = \mathbf{AQ} = \mathbf{PAQ} \tag{2.16}$$

we can write

$$\widehat{\mathbf{r}}_n = \mathbf{P}(\mathbf{b} - \mathbf{A}\mathbf{x}_0) - \mathbf{PA}(\widehat{\mathbf{x}}_n - \mathbf{x}_0) = \widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}(\widehat{\mathbf{x}}_n - \mathbf{x}_0) \in \widehat{\mathbf{r}}_0 + \widehat{\mathbf{A}}\widehat{\mathcal{K}}_n\,.$$

Thus, instead of (2.15) we can solve the equivalent singular system

$$\widehat{\mathbf{A}}(\widehat{\mathbf{x}} - \mathbf{x}_0) = \widehat{\mathbf{r}}_0 \tag{2.17}$$

subject to $\widehat{\mathbf{x}} - \mathbf{x}_0 \in (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$. Obviously, the most straightforward approach is to start the iteration with $\widehat{\mathbf{x}}_0 = \mathbf{x}_0$ and to build up the nested sequence of Krylov subspaces

$$\widehat{\mathcal{K}}_n := \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) := \mathsf{span}\,\{\widehat{\mathbf{r}}_0, \widehat{\mathbf{A}}\widehat{\mathbf{r}}_0, \ldots, \widehat{\mathbf{A}}^{n-1}\widehat{\mathbf{r}}_0\} \subseteq (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp} \tag{2.18}$$

in accordance with the second condition in (2.4). Moreover, since we are heading for BiCG, the first choice for $\widehat{\mathcal{L}}_n$ will be the dual space of $\widehat{\mathcal{K}}_n$, namely,

$$\widehat{\mathcal{L}}_n := \mathcal{K}_n(\widehat{\mathbf{A}}^{\mathsf{H}}, \widehat{\widetilde{\mathbf{y}}}_0) := \mathsf{span}\,\{\widehat{\widetilde{\mathbf{y}}}_0, \widehat{\mathbf{A}}^{\mathsf{H}}\widehat{\widetilde{\mathbf{y}}}_0, \ldots, (\widehat{\mathbf{A}}^{\mathsf{H}})^{n-1}\widehat{\widetilde{\mathbf{y}}}_0\} \subseteq \mathcal{U}^{\perp} \tag{2.19}$$

with a suitable $\widehat{\widetilde{\mathbf{y}}}_0 \perp \mathcal{U}$, which may be the projection of an initial residual $\widetilde{\mathbf{r}}_0$ of a dual problem; see section 4. Later we will come across other suitable choices satisfying

$$\widehat{\mathcal{K}}_n \subseteq \mathcal{R}(\widehat{\mathbf{A}}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp} \qquad \text{and} \qquad \widehat{\mathcal{L}}_n \subseteq \mathcal{R}(\widehat{\mathbf{A}}^{\mathsf{H}}) = \mathcal{U}^{\perp}\,. \tag{2.20}$$

So, the choice (2.18), (2.19) should just be considered as the basic example that fits into our framework.

Remark 2.2. Although $\widehat{\mathbf{r}}_0 \in (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ and $\mathcal{R}(\widehat{\mathbf{A}}) = \mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$, and thus $\widehat{\mathcal{K}}_n \subseteq (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$, we cannot be sure that $\widehat{\mathbf{A}}\big|_{(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}}$ is nonsingular. In fact, $\mathcal{N}(\widehat{\mathbf{A}}) = \mathcal{U}$ and $\mathcal{R}(\widehat{\mathbf{A}})$ may have a nontrivial intersection. In other words, when solving the singular system (2.17) by a Krylov subspace method fully restricted to $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ we may still apply it to a singular system, whence even GMRes may break down; see e.g., [10, 25] and, regarding breakdowns in deflation methods, [11, 28, 32]. However, if $\mathcal{U}$ and $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$ indeed approximate the right invariant subspace of $\mathbf{A}$ and the left invariant subspace of $\overline{\mathbf{A}}$ (the complex conjugate of $\mathbf{A}$), respectively, which belong to

the small eigenvalues of $\mathbf{A}$, it is most likely that $\widehat{\mathbf{A}}\big|_{(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}}$ is nonsingular. For the case of exactly invariant subspaces, see section 7, in particular Corollary 7.2.

Remark 2.3. In contrast to the possibly nontrivial intersection of $\mathcal{R}(\widehat{\mathbf{A}})$ and $\mathcal{U}$ we have $\mathcal{R}(\widehat{\mathbf{A}}) \cap \mathcal{Z} = \{\mathbf{0}\}$. In fact, $\mathcal{R}(\widehat{\mathbf{A}}) \cap \mathcal{Z} = \mathcal{R}(\mathbf{P}) \cap \mathcal{N}(\mathbf{P}) = \{\mathbf{0}\}$ because $\mathbf{P}$ is a projector.

Remark 2.4. Note that even when $\widetilde{\mathbf{U}} = \mathbf{U}$ and $\widehat{\mathcal{K}}_n = \widehat{\mathcal{L}}_n$ the assumptions of Theorem 2.1 are more general than those in the corresponding Theorem 3.2 of [28] since $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ need not be Krylov subspaces here.

3. Deflated BiCG. The iterates $\mathbf{x}_n$ and their residuals $\mathbf{r}_n$ of BiCG are mathematically characterized by relations of the form (1.1) with $\mathbf{B} = \mathbf{I}$ and

$$\mathcal{S}_n = \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,, \qquad \widetilde{\mathcal{S}}_n = \mathcal{K}_n(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{y}}_0)\,, \tag{3.1}$$

where[6] $\widetilde{\mathbf{y}}_0$ has to satisfy $\langle \widetilde{\mathbf{y}}_0, \mathbf{B}\mathbf{r}_0\rangle \neq 0$. This choice allows for the existence of three-term recurrences (or pairs of coupled two-term recurrences) for these iterates and residuals.

As pointed out in [29] and [30], the BiCG method can be generalized to include a formal inner product matrix $\mathbf{B}$, but for the short recursions to persist we need that $\mathbf{B}$ commutes with $\mathbf{A}$, that is, $\mathbf{BA} = \mathbf{AB}$. An implementation of this generalized BiCG (GenBiCG) method can be obtained from any BiCG algorithm by replacing the Euclidean inner product $\langle \widetilde{\mathbf{y}}, \mathbf{y}\rangle = \widetilde{\mathbf{y}}^{\mathsf{H}}\mathbf{y}$ by a formal $\mathbf{B}$-inner product $\langle \widetilde{\mathbf{y}}, \mathbf{y}\rangle_{\mathbf{B}} := \langle \widetilde{\mathbf{y}}, \mathbf{B}\mathbf{y}\rangle = \widetilde{\mathbf{y}}^{\mathsf{H}}\mathbf{B}\mathbf{y}$. The special case $\mathbf{B} := \mathbf{A}$ of the method has recently been introduced as the biconjugate residual (BiCR) method by Sogabe, Sugihara, and Zhang [50, 51]. They optimized the recurrences for this case and showed by numerical experiments that this method converges typically smoother than BiCG. Since then, BiCR and related methods such as BiCRStab have become popular in China and Japan; see, e.g., [3, 4, 33, 64].

In n steps a BiCG or GenBiCG algorithm generates a basis $\{\mathbf{r}_0, \ldots, \mathbf{r}_n\}$ of $\mathcal{K}_{n+1}(\mathbf{A}, \mathbf{r}_0)$ consisting of residual vectors and a basis $\{\widetilde{\mathbf{y}}_0, \ldots, \widetilde{\mathbf{y}}_n\}$ of $\mathcal{K}_{n+1}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{y}}_0)$ in such a way that $\langle \widetilde{\mathbf{y}}_k, \mathbf{B}\mathbf{r}_l\rangle = 0$ if $k \neq l$ and $\langle \widetilde{\mathbf{y}}_k, \mathbf{B}\mathbf{r}_k\rangle \neq 0$. Such bases are called *biorthogonal* or, if $\langle \widetilde{\mathbf{y}}_k, \mathbf{B}\mathbf{r}_l\rangle = \delta_{k,l}$ (with the Kronecker δ), *biorthonormal* or *dual*. (In our terminology we drop the dependence on $\mathbf{B}$.) The vectors $\widetilde{\mathbf{y}}_0, \ldots, \widetilde{\mathbf{y}}_n$ are often referred to as *shadow residuals*. They may be chosen as unit vectors unless we want to solve at once a pair of dual linear systems $\mathbf{Ax} = \mathbf{b}$ and $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$; see section 4. For GenBiCG not to break down we need $\langle \widetilde{\mathbf{y}}_n, \mathbf{B}\mathbf{r}_n\rangle \neq 0$ and $\langle \widetilde{\mathbf{y}}_n, \mathbf{AB}\mathbf{r}_n\rangle \neq 0$ for all n till convergence. Otherwise, there will be a Lanczos breakdown or a pivot breakdown, respectively. These are rare, however, and, except for the extremely rare occasion of an incurable breakdown, they can be avoided with look-ahead techniques; see, e.g., [24, 30].

To find augmented and deflated BiCG and GenBiCG methods we still start from (1.1) but now choose $\mathcal{S}$ and $\widetilde{\mathcal{S}}$ of the structure (2.1) with $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ as in (2.18) and (2.19). For generating these subspaces with the non-Hermitian Lanczos process we will need that $\widehat{\mathbf{A}}\mathbf{B} = \mathbf{B}\widehat{\mathbf{A}}$ on $\mathcal{R}(\widehat{\mathbf{A}}) = \mathcal{R}(\mathbf{P})$, that is, $\widehat{\mathbf{A}}\mathbf{B}\mathbf{P} = \mathbf{B}\widehat{\mathbf{A}}\mathbf{P}$. Therefore, we will assume that $\mathbf{B}$ commutes with $\mathbf{A}$ and $\mathbf{P}$. In particular, $\mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$ must then be an invariant subspace of $\mathbf{B}$, which is a severe restriction unless $\mathbf{B} = \mathbf{I}$.

[6] Many authors use the notation $\widetilde{\mathbf{r}}_0$ instead of $\widetilde{\mathbf{y}}_0$ even if this starting vector does not come from a residual of a dual system—the case we will treat in section 4. However, here in sections 3 and 4 we want to distinguish between these two cases.

As before, we could represent $\mathbf{x}_n$ and $\mathbf{r}_n$ as in (2.2) and (2.3), and $\widetilde{\mathbf{y}}_n$ by, say,

$$\widetilde{\mathbf{y}}_n = \left(\widetilde{\mathbf{y}}_0 - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{V}}_n\widetilde{\mathbf{c}}_n - \widetilde{\mathbf{Z}}\widetilde{\mathbf{u}}_n\right)/\widetilde{\eta}_n\,, \tag{3.2}$$

where the scalar $\widetilde{\eta}_n$ can be chosen to scale $\widetilde{\mathbf{y}}_n$. These representations could be used to derive recursions for $\mathbf{x}_n$, $\mathbf{r}_n$, and $\widetilde{\mathbf{y}}_n$; however, they are not needed since Theorem 2.1 holds: we can apply BiCG or GenBiCG to the singular system $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$ and, after convergence, use the correction formula (2.14) to obtain $\mathbf{x}_n$. Using this implicit approach, these methods can be implemented in the very simple way that is outlined in Algorithm 1 for deflated GenBiCG. For deflated BiCG choose $\mathbf{B} = \mathbf{I}$. By construction, the initial projected residual $\widehat{\mathbf{r}}_0$ lies in the range of $\widehat{\mathbf{A}}$. The initial shadow residual $\widetilde{\mathbf{y}}_0$ gets projected into the range of $\widehat{\mathbf{A}}^{\mathsf{H}}$ by setting $\widehat{\widetilde{\mathbf{y}}}_0 := \mathbf{Q}^{\mathsf{H}}\widetilde{\mathbf{y}}_0$.

```
1 function [n, x_n, r_n] = DeflGenBiCG(A, B, b, x_0, ỹ_0, U, Ũ)
  input  : b, x_0, ỹ_0, U, Ũ;
           code for A, A^H, B, B^H, M, M^H, P, Q, Q^H, Â, Â^H;
                                                        [see Table 1]
  output: approximate solution x_n of Ax = b; corresponding n, r_n;
2 r_0 := b − Ax_0;   r̂_0 := P r_0;   ỹ̂_0 := Q^H ỹ_0;   h_0 := 0;
3 [n, h_n, r̂_n] = GenBiCG(Â, B, r̂_0, h_0, ỹ̂_0);     [apply GenBiCG to Âh = r̂_0]
4 x̂_n := h_n + x_0;   x_n := Qx̂_n + MBb;   r_n := r̂_n;          [see eqn. (2.14)]
```

Algorithm 1: DeflGenBiCG. This outline of our augmented and deflated GenBiCG algorithm for solving $\mathbf{Ax} = \mathbf{b}$ illustrates the application of Theorem 2.1 when the basic method is GenBiCG, which is assumed to be implemented in `function` $[n, \mathbf{x}_n, \mathbf{r}_n] = \texttt{GenBiCG}(\mathbf{A}, \mathbf{B}, \mathbf{b}, \mathbf{x}_0, \widetilde{\mathbf{y}}_0)$ for a system of the form $\mathbf{Ax} = \mathbf{b}$, using the initial approximation $\mathbf{x}_0$ and the initial shadow residual $\widetilde{\mathbf{y}}_0$.

Note that in the Hermitian case of deflated BiCG, where $\mathbf{A} = \mathbf{A}^{\mathsf{H}}$, $\mathbf{B} = \mathbf{I}$, $\widetilde{\mathcal{U}} = \mathcal{U}$, and $\widehat{\mathcal{L}}_n = \widehat{\mathcal{K}}_n$, the conditions (2.12) turn into those of deflated CG. This is not true for the recycling BiCG method proposed by Ahuja [5]. In our notation, that method defines $\widehat{\mathbf{A}} := \mathbf{PAP}$ with $\mathbf{P} := \mathbf{P}_{\mathbf{A}} := \mathbf{I} - \mathbf{AMA}$ based on the choice $\mathbf{B} = \mathbf{A}$, and it then uses the Petrov–Galerkin conditions

$$\mathbf{r}_n \perp \widehat{\mathcal{L}}_n + \widetilde{\mathcal{Z}}\,, \qquad \widetilde{\mathbf{r}}_n \perp \widehat{\mathcal{K}}_n + \mathcal{Z}\,. \tag{3.3}$$

In particular, $\mathbf{r}_n$ is not orthogonal to the shadow search space for the approximate solutions; the Petrov–Galerkin conditions (3.3) are not instances of our conditions $\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{S}}_n$ and $\widetilde{\mathbf{r}}_n \perp \mathbf{B}\mathcal{S}_n$ in (1.1) and (4.2) below, respectively. Instead, Ahuja [5] makes use of two different formal inner products when setting up the Petrov–Galerkin conditions for the two parts of the test spaces.

If $\widetilde{\mathcal{U}} = \mathcal{U}$ and $\widehat{\mathcal{L}}_n = \widehat{\mathcal{K}}_n (\forall n)$, our framework reduces to the one of [28]. Some basic facts about the methods covered in this section and in [28] are compiled in Table 2.

4. Solving pairs of dual linear systems. The non-Hermitian (or two-sided) Lanczos process and BiCG make use of duality. For $n = 1, 2, \ldots$ until it terminates or breaks down, the (generalized) Lanczos process generates dual (or at least biorthogonal) bases $\{\mathbf{y}_0, \ldots, \mathbf{y}_{n-1}\}$ and $\{\widetilde{\mathbf{y}}_0, \ldots, \widetilde{\mathbf{y}}_{n-1}\}$ for the Krylov subspaces $\mathcal{K}_n(\mathbf{A}, \mathbf{y}_0)$ and $\mathcal{K}_n(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{y}}_0)$, respectively. The replacement of $\mathbf{y}_k$ by the residual $\mathbf{r}_k$ is just a question

TABLE 2

The formal inner product matrix $\mathbf{B}$ *and the subspaces* $\widehat{\mathcal{K}}_n$ *and* $\widehat{\mathcal{L}}_n$ *for the methods of section* 3 *and for some of the methods of* [28]. *Note that* $\mathbf{B}$ *in* [28] *corresponds to our* $\mathbf{B}^{\mathsf{H}}$. *On the first two lines,* $\widehat{\widetilde{\mathbf{y}}}_0 := \mathbf{Q}^{\mathsf{H}}\widetilde{\mathbf{y}}_0$, *where* $\widetilde{\mathbf{y}}_0$ *is any suitably chosen initial shadow residual. In the case where we also solve a dual problem* $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$ *(see section* 4), $\widetilde{\mathbf{y}}_0 := \widetilde{\mathbf{r}}_0 := \widetilde{\mathbf{b}} - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}}_0$ *is the initial residual of the dual problem. In this latter case, deflated* GENBICG *with* $\mathbf{B} \neq \mathbf{I}$ *will additionally require generating yet another pair of sequences of Krylov subspaces. Except for deflated* GMRES *and the deflated version of the generalized conjugate residual* (GCR) *method* [15], *all the methods listed in the table can be implemented with three-term or coupled two-term recurrences.*

Method	$\mathbf{B}$	$\widetilde{\mathbf{U}}$	$\widehat{\mathcal{K}}_n$	$\widehat{\mathcal{L}}_n$	Requirements
Deflated BICG	$\mathbf{I}$	$\widetilde{\mathbf{U}}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}^{\mathsf{H}}, \widehat{\widetilde{\mathbf{y}}}_0)$	–
Deflated GENBICG	$\mathbf{B}$	$\widetilde{\mathbf{U}}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}^{\mathsf{H}}, \widehat{\widetilde{\mathbf{y}}}_0)$	$\widehat{\mathbf{A}}\mathbf{B}\mathbf{P} = \mathbf{B}\widehat{\mathbf{A}}\mathbf{P}$
Deflated CG	$\mathbf{I}$	$\mathbf{U}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathbf{A}$ Hpd
Deflated CR	$\mathbf{A}$	$\mathbf{U}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathbf{A}$ Hpd
Deflated MINRES	$\mathbf{A}$	$\mathbf{U}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathbf{A} = \mathbf{A}^{\mathsf{H}}$
Deflated GMRES, GCR	$\mathbf{A}^{\mathsf{H}}$	$\mathbf{U}$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	–

of rescaling. To fully profit from duality, we may assume that we have to solve both $\mathbf{A}\mathbf{x} = \mathbf{b}$ and its dual system

$$\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}\,. \tag{4.1}$$

We denote by $\widetilde{\mathbf{x}}_n$ its approximate solutions and by $\widetilde{\mathbf{r}}_n := \widetilde{\mathbf{b}} - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}}_n$ the corresponding residuals. An example for the occurrence of pairs of dual systems in practice is interpolatory model reduction; see, e.g., [6, 9]. A simple extension of BICG, which is based on coupled two-term recursions for the non-Hermitian Lanczos process, allows us to solve both systems at once at the cost of two matvecs per search space dimension, one with $\mathbf{A}$ and one with $\mathbf{A}^{\mathsf{H}}$. So, essentially the cost is the same as solving just one system with BICG. The iterates $\widetilde{\mathbf{x}}_n$ of the dual system are mathematically characterized by

$$\widetilde{\mathbf{x}}_n \in \widetilde{\mathbf{x}}_0 + \widetilde{\mathcal{S}}_n\,, \qquad \widetilde{\mathbf{r}}_n \in \widetilde{\mathbf{r}}_0 + \mathbf{A}^{\mathsf{H}}\widetilde{\mathcal{S}}_n\,, \qquad \widetilde{\mathbf{r}}_n \perp \mathbf{B}\mathcal{S}_n \tag{4.2}$$

with $\mathcal{S}_n$ and $\widetilde{\mathcal{S}}_n$ as in (3.1), except that we have to choose $\widetilde{\mathbf{y}}_0 := \widetilde{\mathbf{r}}_0$. That is, the residuals $\widetilde{\mathbf{r}}_n$ of the dual system replace the shadow residuals $\widetilde{\mathbf{y}}_n$ of BICG.

In this section we aim at solving a pair of dual systems efficiently with a suitable deflation and augmentation method, as Ahuja [5] did, and our natural targets are deflated BICG and GENBICG. To this end we first address the question of how to solve the dual problem by deflated BICG or GENBICG, and then we hope to solve both the basic and the dual systems at essentially the price of solving one.

To solve the dual system, we start from (4.2) (instead of (1.1)) choosing $\widetilde{\mathcal{S}}$ and $\mathcal{S}$ of the structure

$$\widetilde{\mathcal{S}}_n = \widetilde{\mathcal{L}}_n + \widetilde{\mathcal{U}}\,, \qquad \mathcal{S}_n = \widetilde{\mathcal{K}}_n + \mathcal{U} \tag{4.3}$$

with Krylov subspaces $\widetilde{\mathcal{L}}_n$ and $\widetilde{\mathcal{K}}_n$ that still need to be specified. So, for the dual problem the solution search space is $\widetilde{\mathcal{S}}_n$, and its Krylov subspace is $\widetilde{\mathcal{L}}_n$ (since it is a "left-hand side" Krylov subspace generated by $\mathbf{A}^{\mathsf{H}}$), while the test space is $\mathcal{S}_n$ and its Krylov subspace is $\widetilde{\mathcal{K}}_n$. Analogously to (2.2) and (2.3) we represent the iterates and

residuals of the dual linear system as

$$\widetilde{\mathbf{x}}_n = \widetilde{\mathbf{x}}_0 + \widetilde{\mathbf{V}}_n\widetilde{\mathbf{c}}_n + \widetilde{\mathbf{U}}\widetilde{\mathbf{u}}_n\,, \tag{4.4}$$

$$\widetilde{\mathbf{r}}_n = \widetilde{\mathbf{r}}_0 - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{V}}_n\widetilde{\mathbf{c}}_n - \widetilde{\mathbf{Z}}\widetilde{\mathbf{u}}_n \tag{4.5}$$

with coordinate vectors $\widetilde{\mathbf{c}}_n \in \mathbb{C}^n$ and $\widetilde{\mathbf{u}}_n \in \mathbb{C}^k$, where now the columns of $\widetilde{\mathbf{V}}_n$ form a basis of $\widetilde{\mathcal{L}}_n$. To define a projected problem that yields the appropriate splitting of the search spaces for any $\mathbf{B}$ that commutes with $\mathbf{A}$ and $\mathbf{P}$, we let

$$\widetilde{\mathbf{E}} := \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{U}}\,, \qquad \widetilde{\mathbf{M}} := \widetilde{\mathbf{U}}\widetilde{\mathbf{E}}^{-1}\mathbf{U}^{\mathsf{H}}, \tag{4.6}$$

assuming that $\widetilde{\mathbf{E}}$ is nonsingular, and then define

$$\widetilde{\mathbf{P}} := \mathbf{I} - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{M}}\mathbf{B}^{\mathsf{H}}\,, \qquad \widetilde{\mathbf{Q}} := \mathbf{I} - \widetilde{\mathbf{M}}\mathbf{B}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\,; \tag{4.7}$$

see Table 1. $\widetilde{\mathbf{P}}$ is the oblique projection on $(\mathbf{B}\mathcal{U})^{\perp}$ along $\widetilde{\mathcal{Z}}$, and $\widetilde{\mathbf{Q}}$ is the oblique projection on $(\mathbf{AB}\mathcal{U})^{\perp}$ along $\widetilde{\mathcal{U}}$. Note that due to the commutativity assumption $\widetilde{\mathbf{E}} = \mathbf{E}^{\mathsf{H}}$, $\widetilde{\mathbf{M}} = \mathbf{M}^{\mathsf{H}}$ and $\mathcal{R}(\mathbf{Q}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{Z}})^{\perp}$, $\mathcal{R}(\widetilde{\mathbf{Q}}) = (\mathbf{B}\mathcal{Z})^{\perp}$ now. Finally, we need to introduce iterates and residuals for the corresponding projected dual linear system:

$$\widehat{\widetilde{\mathbf{x}}}_n := \widetilde{\mathbf{x}}_0 + \widetilde{\mathbf{V}}_n\widetilde{\mathbf{c}}_n \in \widetilde{\mathbf{x}}_0 + \widetilde{\mathcal{L}}_n\,, \qquad \widehat{\widetilde{\mathbf{r}}}_n := \widetilde{\mathbf{P}}(\widetilde{\mathbf{b}} - \mathbf{A}^{\mathsf{H}}\widehat{\widetilde{\mathbf{x}}}_n)\,; \tag{4.8}$$

in particular, $\widehat{\widetilde{\mathbf{x}}}_0 := \widetilde{\mathbf{x}}_0$ and $\widehat{\widetilde{\mathbf{r}}}_0 := \widetilde{\mathbf{P}}\widetilde{\mathbf{r}}_0 \perp \mathbf{B}\mathcal{U}$. Then the following analogue of Theorem 2.1 can be quickly established.

THEOREM 4.1. *Modify the assumptions of Theorem* 2.1 *by now letting* $\widetilde{\mathbf{E}} := \mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{U}}$ (*instead of* $\mathbf{E}$) *be nonsingular, so that the matrices* $\widetilde{\mathbf{M}}, \widetilde{\mathbf{P}}, \widetilde{\mathbf{Q}}$ *of* (4.6) *and* (4.7) *are well defined. Then the two pairs of conditions*

$$\widetilde{\mathbf{x}}_n \in \widetilde{\mathbf{x}}_0 + \widetilde{\mathcal{L}}_n + \widetilde{\mathcal{U}}\,, \qquad \widetilde{\mathbf{r}}_n \perp \mathbf{B}(\widetilde{\mathcal{K}}_n + \mathcal{U}) \tag{4.9}$$

and

$$\widehat{\widetilde{\mathbf{x}}}_n \in \widetilde{\mathbf{x}}_0 + \widetilde{\mathcal{L}}_n\,, \qquad \widehat{\widetilde{\mathbf{r}}}_n \perp \mathbf{B}\widetilde{\mathcal{K}}_n\,, \tag{4.10}$$

if determining $\widetilde{\mathbf{x}}_n$ *and* $\widehat{\widetilde{\mathbf{x}}}_n$ *uniquely, are equivalent in the sense that*

$$\widetilde{\mathbf{x}}_n = \widetilde{\mathbf{Q}}\widehat{\widetilde{\mathbf{x}}}_n + \widetilde{\mathbf{M}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{b}} \quad \textit{and} \quad \widetilde{\mathbf{r}}_n = \widehat{\widetilde{\mathbf{r}}}_n\,. \tag{4.11}$$

Hence, again we can either directly aim at $\widetilde{\mathbf{x}}_n$ and $\widetilde{\mathbf{r}}_n$ satisfying (4.9) or first compute $\widehat{\widetilde{\mathbf{x}}}_n$, $\widehat{\widetilde{\mathbf{r}}}_n$ satisfying (4.10) and then apply (4.11). The proof of Theorem 4.1 is fully analogous to that of Theorem 2.1.

Now, recall that $\widehat{\widetilde{\mathbf{r}}}_n$ is the residual of the approximate solution $\widehat{\widetilde{\mathbf{x}}}_n$ of the system

$$\widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}}\widehat{\widetilde{\mathbf{x}}} = \widetilde{\mathbf{P}}\widetilde{\mathbf{b}}\,, \tag{4.12}$$

which is equivalent to

$$\widetilde{\mathbf{A}}(\widehat{\widetilde{\mathbf{x}}} - \widetilde{\mathbf{x}}_0) = \widehat{\widetilde{\mathbf{r}}}_0\,, \qquad \text{where} \quad \widetilde{\mathbf{A}} := \widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}} = \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{Q}} = \widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{Q}} \tag{4.13}$$

(cf. Table 1). Here both sides of the system lie in $\mathcal{R}(\widetilde{\mathbf{P}}) = (\mathbf{B}\mathcal{U})^{\perp}$, and, by assumption, $\widehat{\widetilde{\mathbf{x}}}_n - \widehat{\widetilde{\mathbf{x}}}_0 \in \widetilde{\mathcal{L}}_n$. We want to solve (4.12) by a Krylov subspace method restricted to

$(\mathbf{B}\mathcal{U})^{\perp}$ and, hence, we aim for $\widetilde{\mathcal{L}}_n \subseteq (\mathbf{B}\mathcal{U})^{\perp}$. Obviously, for solving the projected dual system, the natural choice for the Krylov search subspaces is

$$\widetilde{\mathcal{L}}_n := \mathcal{K}_n(\widetilde{\mathbf{A}}, \widehat{\widetilde{\mathbf{r}}}_0) = \mathcal{K}_n(\widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}}, \widehat{\widetilde{\mathbf{r}}}_0) \subseteq (\mathbf{B}\mathcal{U})^{\perp}\,. \tag{4.14}$$

We conclude that for solving $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$ by an augmented and deflated GenBiCG method there are, for given $\mathbf{A}$, $\mathbf{B}$, $\mathbf{U}$, and $\widetilde{\mathbf{U}}$, well-defined projections $\widetilde{\mathbf{P}}$, $\widetilde{\mathbf{Q}}$ and a corresponding projected singular operator $\widetilde{\mathbf{A}}$ that allow us to solve instead of $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$ the deflated system $\widetilde{\mathbf{A}}(\widehat{\widetilde{\mathbf{x}}} - \widetilde{\mathbf{x}}_0) = \widehat{\widetilde{\mathbf{r}}}_0$. Constructing $\widehat{\widetilde{\mathbf{x}}}_n$ and $\widehat{\widetilde{\mathbf{r}}}_n := \widetilde{\mathbf{P}}(\widetilde{\mathbf{b}} - \mathbf{A}^{\mathsf{H}}\widehat{\widetilde{\mathbf{x}}}_n)$ with GenBiCG using only short recurrences requires in particular computing in addition to the basis vectors $\widehat{\widetilde{\mathbf{r}}}_l$ of $\widetilde{\mathcal{L}}_n$ a set of dual basis vectors $\widehat{\mathbf{y}}_k$ of the dual Krylov subspace

$$\widetilde{\mathcal{K}}_n := \mathcal{K}_n(\widetilde{\mathbf{A}}^{\mathsf{H}}, \widehat{\mathbf{y}}_0) = \mathcal{K}_n(\mathbf{A}\widetilde{\mathbf{P}}^{\mathsf{H}}, \widehat{\mathbf{y}}_0) \subseteq \widetilde{\mathcal{U}}^{\perp} \tag{4.15}$$

with $\widehat{\mathbf{y}}_0 \in \widetilde{\mathcal{U}}^{\perp}$ and $\langle \widehat{\widetilde{\mathbf{r}}}_l, \mathbf{B}\widehat{\mathbf{y}}_k \rangle = \delta_{l,k}$. Here, $\mathbf{B}^{\mathsf{H}}$ must commute with $\widetilde{\mathbf{A}}$. This means that $\mathbf{B}$ must commute with $\mathbf{A}$ and $\widetilde{\mathbf{P}}^{\mathsf{H}}$.

We are free to choose $\widehat{\mathbf{y}}_0 := \widehat{\mathbf{r}}_0$ and $\widehat{\widetilde{\mathbf{y}}}_0 := \widehat{\widetilde{\mathbf{r}}}_0$, but, in general, we will still have $\widehat{\mathcal{K}}_n \neq \widehat{\widetilde{\mathcal{K}}}_n$ and $\widehat{\mathcal{L}}_n \neq \widehat{\widetilde{\mathcal{L}}}_n$ if $\mathbf{B} \neq \mathbf{I}$. So, in general, for solving both the basic and the dual problems by an augmented and deflated GenBiCG method we need to build up four Krylov subspaces:

$$\widehat{\mathcal{K}}_n := \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)\,, \quad \widehat{\mathcal{L}}_n := \mathcal{K}_n(\widehat{\mathbf{A}}^{\mathsf{H}}, \widehat{\widetilde{\mathbf{y}}}_0)\,, \quad \widetilde{\mathcal{L}}_n := \mathcal{K}_n(\widetilde{\mathbf{A}}, \widehat{\widetilde{\mathbf{r}}}_0)\,, \quad \widetilde{\mathcal{K}}_n := \mathcal{K}_n(\widetilde{\mathbf{A}}^{\mathsf{H}}, \widehat{\mathbf{y}}_0)\,. \tag{4.16}$$

This means that, in general, the computational cost of building up these Krylov subspaces, that is, for generating the iterates and residuals, is twice as much as we would have hoped for since only $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ and $\mathcal{K}_n(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0)$ are needed for nondeflated BiCG and GenBiCG. Fortunately, in the case $\mathbf{B} = \mathbf{I}$ of BiCG this cost reduces again to half, as the following simple result shows.

THEOREM 4.2. *If* $\mathbf{B} = \mathbf{I}$*, the equalities*

$$\mathbf{P}^{\mathsf{H}} = \widetilde{\mathbf{Q}}\,, \qquad \mathbf{Q}^{\mathsf{H}} = \widetilde{\mathbf{P}}$$

hold, and hence

$$\widehat{\mathbf{A}}^{\mathsf{H}} = \widetilde{\mathbf{A}}\,.$$

Therefore, if we choose $\widehat{\widetilde{\mathbf{y}}}_0 := \widehat{\widetilde{\mathbf{r}}}_0$ *and* $\widehat{\mathbf{y}}_0 := \widehat{\mathbf{r}}_0$*, the four Krylov subspaces in* (4.16) *reduce to two,* $\widehat{\mathcal{K}}_n = \widetilde{\mathcal{K}}_n$ *and* $\widehat{\mathcal{L}}_n = \widetilde{\mathcal{L}}_n$*.*

Proof. Clearly, $\mathbf{P}^{\mathsf{H}} = \mathbf{I} - \mathbf{M}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}} = \mathbf{I} - \widetilde{\mathbf{M}}\mathbf{A}^{\mathsf{H}} = \widetilde{\mathbf{Q}}$ and $\mathbf{Q}^{\mathsf{H}} = \mathbf{I} - \mathbf{A}^{\mathsf{H}}\mathbf{M}^{\mathsf{H}} = \mathbf{I} - \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{M}} = \widetilde{\mathbf{P}}$ yield $\widehat{\mathbf{A}}^{\mathsf{H}} = \mathbf{Q}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}} = \widetilde{\mathbf{P}}\mathbf{A}^{\mathsf{H}} = \widetilde{\mathbf{A}}$. ∎

So, only in the case $\mathbf{B} = \mathbf{I}$ can the residuals of the dual problem serve as the shadow residuals of the basic problem, and vice versa. In other words, only in this case is the deflated dual problem equal to the dual of the deflated problem! Hence, it is not worthwhile to choose $\mathbf{B} \neq \mathbf{I}$ (e.g., deflated BiCR) for solving pairs of dual problems. In summary, using our implicit approach, the deflated and augmented BiCG method can be applied to a pair of dual problems as outlined in Algorithm 2.

5. Block Krylov spaces, deflated block BiCG, and deflated ML(s)BiCG. Our theorems on the equivalence of the explicit and implicit approaches to augmentation and deflation carry over to block Krylov subspace methods based on Galerkin

```
1 function [n, x_n, x̃_n, r_n, r̃_n] = DeflBiCG2(A, b, b̃, x_0, x̃_0, U, Ũ)
  input  : b, b̃, x_0, x̃_0, U, Ũ;
           code for A, A^H, M, M^H, P, P^H, Q, Q^H, Â, Â^H      [see Table 1]
  output: approximate solutions x_n of Ax = b and x̃_n of A^H x̃ = b̃;
           corresponding n, r_n, r̃_n
2 r_0 := b − Ax_0;   r̂_0 := P r_0;   r̃_0 := b̃ − A^H x̃_0;   r̂̃_0 := Q^H r̃_0;
  h_0 := 0;   h̃_0 := 0;
3 [n, h_n, h̃_n, r̂_n, r̂̃_n] = BiCG2(Â, r̂_0, r̂̃_0, h_0, h̃_0);
                                   [apply BiCG to Âh = r̂_0 and Â^H h̃ = r̂̃_0]
4 x̂_n := h_n + x_0;   x_n := Qx̂_n + Mb;   r_n := r̂_n;          [see eqn. (2.14)]
5 x̂̃_n := h̃_n + x̃_0;   x̃_n := P^H x̂̃_n + M^H b̃;   r̃_n := r̂̃_n;   [see eqn. (4.11)]
```

Algorithm 2: DeflBiCG2. This outline of our augmented and deflated BiCG algorithm for simultaneously solving $\mathbf{A}\mathbf{x} = \mathbf{b}$ and $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$ illustrates the application of Theorems 2.1 and 4.1 when the basic method BiCG is at the same time applied to a pair of dual systems. BiCG for such a pair of dual system, $\mathbf{A}\mathbf{x} = \mathbf{b}$ and $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{b}}$, is assumed to be implemented in `function` $[n, \mathbf{x}_n, \widetilde{\mathbf{x}}_n, \mathbf{r}_n, \widetilde{\mathbf{r}}_n] = \texttt{BiCG2}(\mathbf{A}, \mathbf{b}, \widetilde{\mathbf{b}}, \mathbf{x}_0, \widetilde{\mathbf{x}}_0)$, which uses the initial approximations $\mathbf{x}_0$ and $\widetilde{\mathbf{x}}_0$.

or Petrov–Galerkin conditions. We illustrate this claim here by discussing a fairly general version of block BiCG.

Given an $N \times r$ matrix $\mathbf{R}_0$ whose columns $\mathbf{r}_0^{(i)}$ may come from the initial residuals of r given linear systems $\mathbf{A}\mathbf{x}^{(i)} = \mathbf{b}^{(i)}$ $(i = 1, \ldots, r)$, we consider block Krylov subspaces of the form

$$\mathcal{K}_{j;\ell}(\mathbf{A}, \mathbf{R}_0) := \sum_{i=1}^{\ell} \mathcal{K}_{j+1}(\mathbf{A}, \mathbf{r}_0^{(i)}) + \sum_{i=\ell+1}^{r} \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0^{(i)}) \tag{5.1}$$

with $0 \le \ell \le r-1$. Likewise we consider an $N \times s$ matrix $\widetilde{\mathbf{R}}_0$ with columns $\widetilde{\mathbf{r}}_0^{(i)}$ and the corresponding shadow block Krylov subspaces

$$\mathcal{K}_{\widetilde{j};\widetilde{\ell}}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) := \sum_{i=1}^{\widetilde{\ell}} \mathcal{K}_{\widetilde{j}+1}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0^{(i)}) + \sum_{i=\widetilde{\ell}+1}^{s} \mathcal{K}_{\widetilde{j}}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0^{(i)}) \tag{5.2}$$

with $0 \le \widetilde{\ell} \le s-1$. (From now on we denote the initial shadow residuals by $\widetilde{\mathbf{r}}_0^{(i)}$, even if they are not initial residuals of a dual linear system.) These two definitions allow for incomplete blocks. Blocks are complete when $\ell = 0$ or $\widetilde{\ell} = 0$, respectively, and, hence, the first sums in (5.1) and (5.2) are empty. Some algorithms work with complete blocks only, while others create successively bases for all Krylov subspaces $\mathcal{K}_{j;\ell}(\mathbf{A}, \mathbf{R}_0)$ and $\mathcal{K}_{\widetilde{j};\widetilde{\ell}}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$. The latter applies in particular to the so-called *band* Lanczos algorithms, both in the symmetric [45, 22] and the nonsymmetric cases [7, 23].

5.1. Deflated block BiCG and block GenBiCG. Standard treatments of block BiCG [43] assume that $r = s$, but this restriction can (and must) be avoided, because at some point residuals or shadow residuals may turn out to be linearly dependent. A suitable remedy to this deficiency consists in reducing r or s from then

on, a process that is also called deflation; see [7, 36]. For simplicity we assume here that such a deflation of the spanning set is not needed before we are satisfied with the reduction of the residual norm and stop the computation anyway. In other words, we assume that for the iteration numbers n of interest, say, for $1 \le n \le M$, there are well-defined values of j, ℓ and $\widetilde{j}$, $\widetilde{\ell}$ such that $n = jr + \ell = \widetilde{j}s + \widetilde{\ell}$ and

$$\mathsf{dim}\, \mathcal{K}_{j;\ell}(\mathbf{A}, \mathbf{R}_0) = jr + \ell\,, \qquad \mathsf{dim}\, \mathcal{K}_{\widetilde{j};\widetilde{\ell}}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) = \widetilde{j}s + \widetilde{\ell}\,.$$

Here our notation assumes that in (5.1) and (5.2) $\mathcal{K}_0(.,.) := \{\mathbf{0}\}$. Of course, in practice the possible need to deal with nearly linearly dependent residuals or shadow residuals requires extra care, but this topic is not within the scope of this paper.

We also assume that there are Arnoldi-like or Lanczos-like recursions for creating bases of the corresponding block Krylov subspaces. Let $\mathbf{Y}_n$ and $\widetilde{\mathbf{Y}}_n$ be matrices with the first n vectors of these bases. For block BiCG we might aim at making $\mathbf{D}_M := \widetilde{\mathbf{Y}}_M^{\mathsf{H}} \mathbf{B} \mathbf{Y}_M$ diagonal, so that the bases are biorthogonal, as in the band Lanczos process without look-ahead [7, 23]. But there are good reasons to relax the biorthogonality condition (which is, in fact, the Petrov–Galerkin condition) and aim at a matrix $\mathbf{D}$ that is block diagonal only, but well conditioned; this can be enhanced by allowing local pivoting of the basis vectors or even more general linear transformations; see [36]. In either case we may apply our framework by replacing in such a block BiCG the operator $\mathbf{A}$ by $\widehat{\mathbf{A}}$ and by accordingly renaming the nested matrices of the bases as $\widehat{\mathbf{Y}}_n$ and $\widehat{\widetilde{\mathbf{Y}}}_n$, respectively, and renaming the generating block Krylov subspaces as

$$\widehat{\mathcal{K}}_n := \mathcal{R}(\widehat{\mathbf{Y}}_n)\,, \qquad \widehat{\mathcal{L}}_n := \mathcal{R}(\widehat{\widetilde{\mathbf{Y}}}_n)\,. \tag{5.3}$$

Again, for block GenBiCG applied to a pair of dual linear systems we would need to construct two additional sequences of block Krylov subspaces generated by $\widetilde{\mathbf{A}}$ and by $\widetilde{\mathbf{A}}^{\mathsf{H}}$, respectively. Therefore, choosing $\mathbf{B} \ne \mathbf{I}$ for pairs of dual problems will be hardly worth the trouble.

Recall that in section 2 we did not assume that $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ are standard Krylov subspaces, but just that they are subspaces of the same dimension. So now, if we consider any particular system, say, $\mathbf{A}\mathbf{x}^{(i_0)} = \mathbf{b}^{(i_0)}$, and substitute $\mathbf{x} := \mathbf{x}^{(i_0)}$, $\mathbf{b} := \mathbf{b}^{(i_0)}$, we can apply the results of sections 2 and 3, in particular Theorem 2.1. This means that we can implement augmentation and deflation by applying block BiCG to a projected system and afterward apply the usual correction step (2.14). Of course, this applies to each of the r basic systems. Note that, in theory, it makes no difference whether we solve just one or all r basic systems, and that there is no need to assume that initially $r = s$.

5.2. Deflated ML(s)BiCG. In principle, even if just one system has to be solved, we could attempt this by choosing for the search space a block Krylov subspace $\mathcal{K}_{j;\ell}(\mathbf{A}, \mathbf{R}_0)$ with $r > 1$ and a matrix $\mathbf{R}_0$ whose first column is the initial residual, while the others are chosen mutually orthogonal. However, we believe that the gain in convergence speed compared to the corresponding ordinary Krylov solver will usually not justify the additional cost and complications of applying a block solver with $r > 1$.

A more promising approach to solving a single system consists in applying a block BiCG algorithm with $r = 1$ and $s > 1$. Such a variation of BiCG called ML(s)BiCG was introduced by Yeung and Chan [61]. For more recent presentations of the method see [59, 60]. The basic idea was to replace the left shadow Krylov subspaces $\mathcal{K}_n(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0)$ of BiCG by block Krylov subspaces that are generated from s linearly independent

initial shadow residuals. Assuming $n = \widetilde{j}s + \widetilde{\ell}$ we can characterize the iterates $\mathbf{x}_n$ of ML(s)BiCG by

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,, \quad \mathbf{r}_n \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,, \quad \mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\mathcal{K}_{\widetilde{j};\widetilde{\ell}}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) \tag{5.4}$$

with $\mathbf{B} = \mathbf{I}$ unless we want to generalize the method. But, unfortunately, a straightforward implementation of ML(s)BiCG is not (yet) competitive due to the high cost of generating s shadow Krylov subspaces. Each step increases the dimension of the search space only by one, but requires $s+1$ matvecs since the dimension of the test space is increased by s. Also, it seems unlikely that such a large test space could speed up the convergence by much, but the results obtained in [59, 60, 61] with the closely related ML(s)BiCGStab method show that it can.

For deflated ML(s)BiCG we use for $\widehat{\mathcal{K}}_n$ the standard choice (2.18) and for $\widehat{\mathcal{L}}_n$, when $n = \widetilde{j}s + \widetilde{\ell}$, the block Krylov subspaces

$$\widehat{\mathcal{L}}_n := \widehat{\mathcal{L}}_{\widetilde{j}s+\widetilde{\ell}} := \mathcal{K}_{\widetilde{j};\widetilde{\ell}}(\widehat{\mathbf{A}}^{\mathsf{H}}, \widetilde{\widehat{\mathbf{R}}}_0) \;\subseteq\; \mathcal{U}^{\perp}\,,$$

where $\widetilde{\widehat{\mathbf{R}}}_0$ must have s linearly independent columns $\widetilde{\widehat{\mathbf{r}}}_0^{(i)} \perp \mathcal{U}$ $(i = 1, \ldots, s)$. (We avoid the notation $\widetilde{\widehat{\mathbf{r}}}_0^{(i)}$ and $\widetilde{\widehat{\mathbf{R}}}_0$ from now on.)

6. Lanczos-type product methods, deflated BiCGStab, and deflated IDR(s). The BiCG and block BiCG methods require the application of $\mathbf{A}^{\mathsf{H}}$, which may make their usage costly or even impossible. It was Sonneveld who introduced with IDR [58] and CGS [52] two methods based on the same glorious idea that allowed him to avoid multiplication by $\mathbf{A}^{\mathsf{H}}$ and, at the same time, to double the degree of the BiCG residual polynomials nearly for free. Van der Vorst's ubiquitous BiCGStab [55], which can be seen to be mathematically equivalent to a version of IDR, makes use of the same idea. Often such methods are called Lanczos-type product methods (LTPMs) now, see, e.g., [30]. Yeung and Chan [59, 60, 61] applied the same idea to their ML(s)BiCG method, which they only introduced as a tool for deriving the more effective and less costly ML(s)BiCGStab method. Sonneveld and van Gijzen's recently generalized the IDR approach to the IDR(s) method [53], which in exact arithmetic can be seen to produce every $s+1$ steps the same approximants as ML(s)-BiCGStab, but is known to be more stable under roundoff. Both ML(s)BiCGStab and IDR(s) reduce mathematically to BiCGStab if $s = 1$. In this section we are going to show how all these methods fit into our framework for deflation and augmentation.

6.1. Deflated BiCGStab and ML(s)BiCGStab. After j full steps of BiCGStab the residual lies in $\mathbf{r}_0 + \mathcal{K}_{2j}(\mathbf{A}, \mathbf{r}_0)$ and will therefore be denoted by $\mathbf{r}_{2j}$ here.[7] This residual is of the product form

$$\mathbf{r}_{2j} = \Omega_j(\mathbf{A})\, \mathbf{r}_j^{\text{BiCG}}\,,$$

where $\mathbf{r}_j^{\text{BiCG}}$ denotes the jth BiCG residual and $\Omega_j(\mathbf{A}) := (\mathbf{I} - \omega_1\mathbf{A}) \cdots (\mathbf{I} - \omega_j\mathbf{A})$ is a polynomial in $\mathbf{A}$ whose parameters ω_k are determined during the iteration by a

[7] In the attempt to fit the methods in our framework, we are using here a numbering of the iterates and residuals that differs from the usual one for BiCGStab and ML(s)BiCGStab. On the other hand, fortunately, it agrees with the standard numbering for IDR(s). But, for example, our odd-numbered BiCGStab residuals $\mathbf{r}_{2j+1}$ correspond to intermediate quantities in the original BiCGStab algorithm.

local residual norm minimization. If we allow for a formal inner product matrix $\mathbf{B}$ that commutes with $\mathbf{A}$, $\mathbf{r}_j^{\text{BiCG}}$ must satisfy

$$\mathbf{r}_j^{\text{BiCG}} \perp \mathbf{B}^{\mathsf{H}}\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0)\,.$$

Consequently, we can say that for BiCGStab the residual $\mathbf{r}_{2j}$ is characterized by

$$\mathbf{r}_{2j} \in \Omega_j(\mathbf{A})\,(\mathbf{r}_0 + \mathbf{A}\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0))\,, \tag{6.1a}$$

$$[\Omega_j(\mathbf{A})]^{-1}\mathbf{r}_{2j} \perp \mathbf{B}^{\mathsf{H}}\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)\,. \tag{6.1b}$$

This is the case $s = 1$, $n = 2j$ of the more general formulas we give next.

For ML(s)BiCGStab, if we let $n = j(s+1) + \ell$, where $0 \le \ell \le s$ and $j = 0, 1, 2, \ldots$, the residuals $\mathbf{r}_n$ are characterized by

$$\mathbf{r}_n \in \Omega_j(\mathbf{A})\,(\mathbf{r}_0 + \mathbf{A}\mathcal{K}_{js+\ell}(\mathbf{A}, \mathbf{r}_0))\,, \tag{6.2a}$$

$$[\Omega_j(\mathbf{A})]^{-1}\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)\,. \tag{6.2b}$$

Both $\mathcal{K}_{js+\ell}(\mathbf{A}, \mathbf{r}_0)$ and $\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$ have, for sufficiently small j, dimension $js + \ell = n - j$. Now, note that (6.2b) is equal to

$$\mathbf{r}_n^{\mathsf{H}}[\Omega_j(\mathbf{A})]^{-\mathsf{H}}\,\mathbf{B}^{\mathsf{H}}\,\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) = \mathbf{0}^{\mathsf{T}}\,,$$

which in turn, again due to the commutativity, can be written as

$$\mathbf{r}_n \perp \mathbf{B}^{\mathsf{H}}\mathcal{L}_n \tag{6.3}$$

with

$$\mathcal{L}_n := \mathcal{L}_{j;\ell} := [\Omega_j(\mathbf{A})]^{-\mathsf{H}}\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) = \mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, [\Omega_j(\mathbf{A})]^{-\mathsf{H}}\widetilde{\mathbf{R}}_0)\,. \tag{6.4}$$

The simple but crucial step from (6.2b) to (6.3)–(6.4) has been pointed out by Simoncini and Szyld [49] in connection with the IDR(s) method (see below). It means that BiCGStab and ML(s)BiCGStab can be viewed as Petrov–Galerkin methods with residual test spaces $\mathcal{L}_n$ that are rational Krylov subspaces, which have dimension $n-j$ (as long as $\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$ is not affected by dimension loss). Alternatively, for each n, they can be viewed as polynomial Krylov subspaces with an initial vector that depends on j. Since we can keep j or even n fixed when applying Theorem 2.1, BiCGStab and ML(s)BiCGStab fit into the general framework of section 2. Deflated versions of these methods are now obtained quickly by replacing $\mathbf{A}$ by $\widehat{\mathbf{A}}$, $\mathbf{r}_0$ by $\widehat{\mathbf{r}}_0$, and by choosing $\widetilde{\mathbf{R}}_0$ such that $\mathcal{R}(\widetilde{\mathbf{R}}_0) \subseteq \mathcal{U}^{\perp}$ in order to define projected search and test spaces $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ for the singular projected linear system (2.17) with the deflated matrix $\widehat{\mathbf{A}}$.

An expression for the solution search space of ML(s)BiCGStab can be found as follows. We define polynomials Ψ_j of degree $j-1$ such that

$$\Omega_j(\mathbf{A}) = \mathbf{I} - \mathbf{A}\Psi_j(\mathbf{A})\,.$$

Then we can rewrite (6.2a) as

$$\mathbf{b} - \mathbf{A}\mathbf{x}_n \in (\mathbf{I} - \mathbf{A}\Psi_j(\mathbf{A}))\,\mathbf{b} - \mathbf{A}\Omega_j(\mathbf{A})\mathbf{x}_0 + \mathbf{A}\Omega_j(\mathbf{A})\mathcal{K}_{js+\ell}(\mathbf{A}, \mathbf{r}_0)\,,$$

which leads to

$$\mathbf{x}_n \in \mathbf{x}_{j;0} + \Omega_j(\mathbf{A})\mathcal{K}_{js+\ell}(\mathbf{A}, \mathbf{r}_0)\,, \qquad \text{where} \quad \mathbf{x}_{j;0} := \Psi_j(\mathbf{A})\mathbf{b} + \Omega_j(\mathbf{A})\mathbf{x}_0\,. \tag{6.5}$$

So, unlike in most other Krylov subspace solvers, the shift vector of the affine solution search space is not constant, but depends on the index j. The same is true for other LTPMs. In particular, BiCGStab is here included as case $s = 1$. This feature reveals a major difference between these methods and classical Galerkin- or Petrov–Galerkin-based Krylov subspace solvers like CG, BiCG, MinRes, GMRes, etc.

6.2. Deflated IDR(s). For $n = j(s+1)$, the IDR(s) residuals do not differ in their mathematical characterization from those of ML(s)BiCGStab. We cover here again a generalization, where $\mathbf{B}$ can be any matrix commuting with $\mathbf{A}$ (while $\mathbf{B} = \mathbf{I}$ in standard IDR(s)). The Petrov–Galerkin condition (6.2b) is relaxed by replacing the test space $\mathcal{K}_{j;\ell}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$ by the smaller space $\mathcal{K}_{j;0}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$:

$$\mathbf{r}_n \in \Omega_j(\mathbf{A})\,(\mathbf{r}_0 + \mathbf{A}\mathcal{K}_{js+\ell}(\mathbf{A}, \mathbf{r}_0))\,, \tag{6.6a}$$

$$[\Omega_j(\mathbf{A})]^{-1}\mathbf{r}_n \;\perp\; \mathbf{B}^{\mathsf{H}}\mathcal{K}_{j;0}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)\,. \tag{6.6b}$$

Consequently, (6.3) persists if (6.4) is replaced by

$$\mathcal{L}_n := \mathcal{L}_{j;\ell} := [\Omega_j(\mathbf{A})]^{-\mathsf{H}}\mathcal{K}_{j;0}(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) = \mathcal{K}_{j;0}(\mathbf{A}^{\mathsf{H}}, [\Omega_j(\mathbf{A})]^{-\mathsf{H}}\widetilde{\mathbf{R}}_0)\,, \tag{6.7}$$

but this characterization does not uniquely define iterates and residuals unless $\ell = 0$. Only in the latter case are they unique, and in fact the same as in ML(s)BiCGStab. Different IDR(s) algorithms [53, 56] may yield for $\ell \neq 0$ different iterates, even in exact arithmetic; the choice is made unique only by the particular form of the recurrences. If we included the corresponding restrictions here, the method would still fit into our framework. The recipe for a deflated IDR(s) is then the same as for ML(s)BiCGStab.

As a summary the spaces $\widehat{\mathcal{K}}_n$ and $\widehat{\mathcal{L}}_n$ that are used to embed the featured methods of sections 5 and 6 into our framework are compiled in Table 3. More could be added. For block BiCG we restrict ourselves here to the classical version [43], where $r = s$.

Table 3
Featured methods of sections 5 *and* 6 *with corresponding subspaces* $\widehat{\mathcal{K}}_n$ *and* $\widehat{\mathcal{L}}_n$ *in the case* $\mathbf{B} = \mathbf{I}$.

Method	$\widehat{\mathcal{K}}_n$	$\widehat{\mathcal{L}}_n$	Requirements
Deflated block BiCG	$\mathcal{K}_{j;\ell}(\widehat{\mathbf{A}}, \mathbf{R}_0)$	$\mathcal{K}_{j;\ell}(\widehat{\mathbf{A}}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$	$n = js + \ell$
Deflated ML(s)BiCG	$\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$	$\mathcal{K}_{j;\ell}(\widehat{\mathbf{A}}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$	$n = js + \ell$
Deflated ML(s)BiCGStab	$\mathcal{K}_{js+\ell}(\widehat{\mathbf{A}}, \Omega_j(\widehat{\mathbf{A}})\mathbf{r}_0)$	$\mathcal{K}_{j;\ell}(\widehat{\mathbf{A}}^{\mathsf{H}}, [\Omega_j(\widehat{\mathbf{A}})]^{-\mathsf{H}}\widetilde{\mathbf{R}}_0)$	$n = j(s+1) + \ell$
Deflated BiCGStab	$\mathcal{K}_{js+\ell}(\widehat{\mathbf{A}}, \Omega_j(\widehat{\mathbf{A}})\mathbf{r}_0)$	$\mathcal{K}_{j;\ell}(\widehat{\mathbf{A}}^{\mathsf{H}}, [\Omega_j(\widehat{\mathbf{A}})]^{-\mathsf{H}}\widetilde{\mathbf{r}}_0)$	$n = 2j + \ell$
Deflated IDR(s)	$\mathcal{K}_{js+\ell}(\widehat{\mathbf{A}}, \Omega_j(\widehat{\mathbf{A}})\mathbf{r}_0)$	$\mathcal{K}_{j;0}(\widehat{\mathbf{A}}^{\mathsf{H}}, [\Omega_j(\widehat{\mathbf{A}})]^{-\mathsf{H}}\widetilde{\mathbf{R}}_0)$	$n = j(s+1) + \ell$

7. Invariant deflation spaces. In this section we discuss the spectral properties of the deflated operator $\widehat{\mathbf{A}} := \mathbf{PA}$ assuming invariant deflation spaces. We extend results of the framework for Galerkin-based methods from [28] to our new framework on Petrov–Galerkin methods.

While our basic equivalence theorem, Theorem 2.1, made no assumption on a relation between $\mathbf{A}$ and $\widehat{\mathbf{A}}$, we have seen that a natural choice for $\widehat{\mathbf{A}}$ is given by (2.16), $\widehat{\mathbf{A}} := \mathbf{PA} = \mathbf{AQ} = \mathbf{PAQ}$. What can we then say about the spectrum of $\widehat{\mathbf{A}}$?

Since the projection $\mathbf{P}$ has the null space $\mathcal{Z} = \mathbf{A}\mathcal{U}$, $\widehat{\mathbf{A}} = \mathbf{PA}$ has the null space $\mathcal{U}$ for any choice of this k-dimensional deflation space. So, the spectrum of $\widehat{\mathbf{A}}$ always contains the eigenvalue zero with algebraic and geometric multiplicity k.

If $\mathcal{U}$ is an invariant subspace of $\mathbf{A}$, then, clearly, the corresponding eigenvalues are moved to zero in the transition to $\widehat{\mathbf{A}}$. But in this case, and in a somewhat dual situation, we can say even more. Let $\mathbf{A}$ have the partitioned Jordan decomposition

$$\mathbf{A} = \mathbf{SJS}^{-1} = \begin{bmatrix} \mathbf{S}_1 & \mathbf{S}_2 \end{bmatrix} \begin{bmatrix} \mathbf{J}_1 & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_2 \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{S}}_1^{\mathsf{H}} \\ \widetilde{\mathbf{S}}_2^{\mathsf{H}} \end{bmatrix}, \tag{7.1}$$

where $\mathbf{S}_1, \widetilde{\mathbf{S}}_1 \in \mathbb{C}^{N\times k}$, $\mathbf{S}_2, \widetilde{\mathbf{S}}_2 \in \mathbb{C}^{N\times(N-k)}$, $\mathbf{J}_1 \in \mathbb{C}^{k\times k}$, and $\mathbf{J}_2 \in \mathbb{C}^{(N-k)\times(N-k)}$. The spectra of $\mathbf{J}_1$ and $\mathbf{J}_2$ need not be disjoint, but in applications of deflation and augmentation methods they most likely are.

Starting from this Jordan form of $\mathbf{A}$, in the following theorem we derive the Jordan form of $\widehat{\mathbf{A}} = \mathbf{PA}$ under the assumption that (1) $\mathcal{U}$ is a right invariant subspace of $\mathbf{A}$ spanned by the columns of $\mathbf{S}_1$, or (2) $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}}$ is a left invariant subspace of $\overline{\mathbf{A}}$ (the complex conjugate of $\mathbf{A}$) spanned by the columns of $\widetilde{\mathbf{S}}_1$, or (3) both assumptions hold.

THEOREM 7.1. *Suppose that the matrix $\mathbf{A} \in \mathbb{C}^{N\times N}$ has a partitioned Jordan decomposition of the form* (7.1)*. Then the following three assertions hold:*

(1) *Assume $\mathcal{U} = \mathcal{R}(\mathbf{S}_1)$, $\mathbf{U} \in \mathbb{C}^{N\times k}$ is any matrix satisfying $\mathcal{R}(\mathbf{U}) = \mathcal{U}$, and $\widetilde{\mathbf{U}} \in \mathbb{C}^{N\times k}$ is such that $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU}$ is nonsingular. Then*

$$\widehat{\mathbf{A}} := \mathbf{PA} = \begin{bmatrix} \mathbf{U} & \mathbf{PS}_2 \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 \end{bmatrix} \begin{bmatrix} \mathbf{U} & \mathbf{PS}_2 \end{bmatrix}^{-1} \tag{7.2}$$

$$\text{with} \quad \begin{bmatrix} \mathbf{U} & \mathbf{PS}_2 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}}(\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}})^{-1} & \widetilde{\mathbf{S}}_2 \end{bmatrix}^{\mathsf{H}}. \tag{7.3}$$

This holds, in particular, for $\mathbf{U} = \mathbf{S}_1$.

(2) *Assume $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$, $\widetilde{\mathbf{U}} \in \mathbb{C}^{N\times k}$ is any matrix satisfying $\mathcal{R}(\widetilde{\mathbf{U}}) = \widetilde{\mathcal{U}}$, and $\mathbf{U} \in \mathbb{C}^{N\times k}$ is such that $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU}$ is nonsingular. Then*

$$\widehat{\mathbf{A}} := \mathbf{PA} = \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 \end{bmatrix} \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix}^{-1} \tag{7.4}$$

$$\text{with} \quad \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}}(\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}})^{-1} & \mathbf{Q}^{\mathsf{H}}\widetilde{\mathbf{S}}_2 \end{bmatrix}^{\mathsf{H}}. \tag{7.5}$$

This holds, in particular, for $\widetilde{\mathbf{U}} = \mathbf{B}^{-\mathsf{H}}\widetilde{\mathbf{S}}_1$.

(3) *Assume $\mathcal{U} = \mathcal{R}(\mathbf{S}_1)$ and $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$. Moreover, let $\mathbf{U} \in \mathbb{C}^{N\times k}$ satisfy $\mathcal{R}(\mathbf{U}) = \mathcal{U}$, and let $\widetilde{\mathbf{U}} \in \mathbb{C}^{N\times k}$ satisfy $\mathcal{R}(\widetilde{\mathbf{U}}) = \widetilde{\mathcal{U}}$. Then $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU}$ is nonsingular and*

$$\widehat{\mathbf{A}} := \mathbf{PA} = \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 \end{bmatrix} \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix}^{-1} \tag{7.6}$$

$$\text{with} \quad \begin{bmatrix} \mathbf{U} & \mathbf{S}_2 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}}(\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}})^{-1} & \widetilde{\mathbf{S}}_2 \end{bmatrix}^{\mathsf{H}}. \tag{7.7}$$

This holds, e.g., for $\mathbf{U} = \mathbf{S}_1$ and $\widetilde{\mathbf{U}} = \mathbf{B}^{-\mathsf{H}}\widetilde{\mathbf{S}}_1$, in which case $\mathbf{U}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathbf{U}} = \mathbf{I}$.

In all three cases the spectrum $\Lambda(\widehat{\mathbf{A}})$ of $\widehat{\mathbf{A}}$ is given by $\Lambda(\widehat{\mathbf{A}}) = \{0\} \cup \Lambda(\mathbf{J}_2)$.

Proof. (1) By assumption, there exists a nonsingular matrix $\mathbf{R} \in \mathbb{C}^{k\times k}$ with $\mathbf{AU} = \mathbf{UR}$. Hence, since $\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU}$ is nonsingular, so is $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BU}$, and $\mathbf{E}^{-1} =$

$\mathbf{R}^{-1}(\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U})^{-1}$. Therefore,

$$\mathbf{P} := \mathbf{I} - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B} = \mathbf{I} - \mathbf{U}(\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U})^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\,. \tag{7.8}$$

Now, recall that $\mathcal{N}(\mathbf{P}) = \mathcal{Z}$ and $\mathcal{R}(\mathbf{P}) = (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$, which translate into

$$\mathbf{P}\mathbf{A}\mathbf{U} = \mathbf{0} \quad \text{and} \quad \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{P} = \mathbf{0}\,,$$

respectively. From (7.8) and the first equation we get

$$\mathbf{P}\mathbf{A}(\mathbf{P}\mathbf{S}_2) = \mathbf{P}\mathbf{A}\left(\mathbf{I} - \mathbf{U}(\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U})^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\right)\mathbf{S}_2 = \mathbf{P}\mathbf{A}\mathbf{S}_2 = (\mathbf{P}\mathbf{S}_2)\mathbf{J}_2\,,$$

which along with $\mathbf{P}\mathbf{A}\mathbf{U} = \mathbf{0}$ will yield (7.2) once we have proven that $\left[\begin{array}{cc}\mathbf{U} & \mathbf{P}\mathbf{S}_2\end{array}\right]$ is nonsingular.

Next, from $\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{S}_1 = \mathbf{0}$ we see that $\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{U} = \mathbf{0}$ and thus, by (7.8), $\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{P} = \widetilde{\mathbf{S}}_2^{\mathsf{H}}$. Collecting $\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{U} = \mathbf{0}$, $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{P} = \mathbf{0}$, and $\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{P}\mathbf{S}_2 = \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{S}_2 = \mathbf{I}$, we obtain altogether

$$\left[\begin{array}{c}(\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U})^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B} \\ \widetilde{\mathbf{S}}_2^{\mathsf{H}}\end{array}\right]\left[\begin{array}{cc}\mathbf{U} & \mathbf{P}\mathbf{S}_2\end{array}\right] = \left[\begin{array}{cc}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}\end{array}\right],$$

which proves the nonsingularity and (7.3).

(2) From $\widetilde{\mathbf{S}}_1^{\mathsf{H}}\mathbf{S}_2 = \mathbf{0}$ and $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$ it follows that $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{S}_2 = \mathbf{0}$. Using the definition of $\mathbf{P}$ and the invariance of $\mathbf{S}_2$, we see that

$$\begin{aligned}\mathbf{P}\mathbf{A}\mathbf{S}_2 &= \left(\mathbf{I} - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\right)\mathbf{A}\mathbf{S}_2 = \mathbf{S}_2\mathbf{J}_2 - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{S}_2\mathbf{J}_2 = \mathbf{S}_2\mathbf{J}_2\,,\\ \mathbf{P}\mathbf{A}\mathbf{U} &= \left(\mathbf{I} - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\right)\mathbf{A}\mathbf{U} = \mathbf{A}\mathbf{U} - \mathbf{A}\mathbf{U}\mathbf{E}^{-1}\mathbf{E} = \mathbf{0}\,,\end{aligned}$$

which yields (7.4) if $\left[\begin{array}{cc}\mathbf{U} & \mathbf{S}_2\end{array}\right]$ is indeed nonsingular.

Indeed, since $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$, there exists a nonsingular $\widetilde{\mathbf{R}} \in \mathbb{C}^{k\times k}$ such that $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A} = \widetilde{\mathbf{R}}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}$. And since $\mathbf{E} = \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\mathbf{U} = \widetilde{\mathbf{R}}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U}$ is nonsingular, so is $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U}$. Moreover, from $\mathcal{N}(\mathbf{Q}) = \mathcal{U}$ we have $\mathbf{Q}\mathbf{U} = \mathbf{0}$, so that

$$\left[\begin{array}{c}(\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U})^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B} \\ \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{Q}\end{array}\right]\left[\begin{array}{cc}\mathbf{U} & \mathbf{S}_2\end{array}\right] = \left[\begin{array}{cc}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{Q}\mathbf{S}_2\end{array}\right].$$

Here, inserting $\mathbf{Q}$ and noting again that $\mathbf{A}\mathbf{S}_2 = \mathbf{S}_2\mathbf{J}_2$ and $\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{S}_2 = \mathbf{0}$, we get

$$\widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{Q}\mathbf{S}_2 = \widetilde{\mathbf{S}}_2^{\mathsf{H}}\left(\mathbf{I} - \mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\right)\mathbf{S}_2 = \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{S}_2 - \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{U}\mathbf{E}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{S}_2\mathbf{J}_2 = \widetilde{\mathbf{S}}_2^{\mathsf{H}}\mathbf{S}_2 = \mathbf{I}\,,$$

which establishes (7.5).

(3) From $\mathcal{U} = \mathcal{R}(\mathbf{S}_1)$ and $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$ we can conclude that for some nonsingular $k \times k$ matrices $\mathbf{R}$, $\mathbf{N}$, and $\widetilde{\mathbf{N}}$ we have

$$\mathbf{E} := \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{A}\mathbf{U} = \widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{B}\mathbf{U}\mathbf{R} = \widetilde{\mathbf{N}}^{\mathsf{H}}\widetilde{\mathbf{S}}_1^{\mathsf{H}}\mathbf{S}_1\mathbf{N}\mathbf{R} = \widetilde{\mathbf{N}}^{\mathsf{H}}\mathbf{N}\mathbf{R}\,.$$

Therefore, $\mathbf{E}$ is nonsingular, as needed. The seeming discrepancy between the formulas (7.2)–(7.7) is resolved by noting that now $\mathbf{P}\mathbf{S}_2 = \mathbf{S}_2$ and $\mathbf{Q}^{\mathsf{H}}\widetilde{\mathbf{S}}_2 = \widetilde{\mathbf{S}}_2$. ∎

There are ways to reformulate the assumptions and conclusions of Theorem 7.1. For example, the assumption $\mathcal{U} = \mathcal{R}(\mathbf{S}_1)$ is equivalent to $\mathcal{U}^\perp = \mathcal{R}(\widetilde{\mathbf{S}}_2)$, and the assumption $\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}} = \mathcal{R}(\widetilde{\mathbf{S}}_1)$ is equivalent to $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp = \mathcal{R}(\mathbf{S}_2)$.

In particular, assertions (2) and (3) of Theorem 7.1 imply the following.

COROLLARY 7.2. *Let* $\widehat{\mathbf{A}} := \mathbf{PA}$ *and assume that* $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp$ *is* $\mathbf{A}$*-invariant. Then* $\mathbf{A}$ *and* $\widehat{\mathbf{A}}$ *are identical when restricted to* $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp$*:*

$$\widehat{\mathbf{A}}\big|_{(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp} = \mathbf{A}\big|_{(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp}. \tag{7.9}$$

Moreover, if also $\mathcal{U}$ *is* $\mathbf{A}$*-invariant, then*

$$\mathcal{U} \oplus (\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp = \mathbb{C}^N \tag{7.10}$$

is the direct decomposition of $\mathbb{C}^N$ *in the null space and range of* $\mathbf{P}$*.*

Proof. The result is a consequence of Theorem 7.1. But it is easy to prove it directly. Assume the $N-k$ columns of $\mathbf{W}$ form a basis of $(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^\perp$. Due to the $\mathbf{A}$-invariance there is a square matrix $\widehat{\mathbf{R}}$ of order $N-k$ such that $\mathbf{AW} = \mathbf{W}\widehat{\mathbf{R}}$. Note that $\mathbf{PW} = \mathbf{W}$ since $\mathbf{P}$ projects on the range of $\mathbf{W}$. Consequently,

$$\widehat{\mathbf{A}}\mathbf{W} = \mathbf{PAW} = \mathbf{PW}\widehat{\mathbf{R}} = \mathbf{W}\widehat{\mathbf{R}} = \mathbf{AW},$$

which proves (7.9).

If also $\mathcal{U}$ is $\mathbf{A}$-invariant, then $\mathcal{U} = \mathcal{Z} = \mathcal{N}(\mathbf{P})$. ∎

Assertions (1) and (2) of Theorem 7.1 generalize Theorem 3.3 of Gaul et al. [28]. As noted there, special cases of those results have appeared in the literature before: for symmetric and positive definite matrices $\mathbf{A}$ and $\mathbf{B} = \mathbf{I}$ in Frank and Vuik [21] and in Nabben and Vuik [39, 40], and for nonsymmetric $\mathbf{A}$ and $\mathbf{B} = \mathbf{I}$ in Erlangga and Nabben [17, 18] and Yeung, Tang and Vuik [62].

The situation of Corollary 7.2 has been aimed at, at least approximately, with the oblique projection $\mathbf{P}$ and the corresponding deflated operator $\widehat{\mathbf{A}} := \mathbf{PAP}$ used in [32].

8. Conclusions. In this paper we introduced a framework for augmented and deflated Krylov subspace methods based on a Petrov–Galerkin condition. This class of methods includes first of all the biconjugate gradient (BiCG) method, but also corresponding block methods and Lanczos-type product methods (LPTMs), including some of today's most competitive methods, such as BiCGStab and IDR(s). We also cover the biconjugate residual (BiCR) method, which is the standard example of a generalized BiCG (GenBiCG) method.

Our basic result is that augmented and deflated variants of all these methods can be realized by just applying the basic, nondeflated method first to a deflated (or projected) linear system, whose matrix is singular, followed by a correction step that must be applied to the resulting approximate solution. This is an implicit way to realize augmentation and deflation; it can be mathematically characterized by the conditions (2.13) and the affine transformation (2.14). For GenBiCG this implicit approach leads immediately to what we list as Algorithm 1 (DeflGenBiCG). Deflated standard BiCG is covered as the special case $\mathbf{B} = \mathbf{I}$. Amazingly, any deflated and augmented LTPM can be implemented in the same way as deflated BiCG: all we need is to replace `GenBiCG` on line 3 of Algorithm 1 by the name of the chosen LTPM code. We also discuss the case where the BiCG or the GenBiCG method is applied to a pair of dual linear systems, where the first has as matrix $\mathbf{A}$ and the other $\mathbf{A}^{\mathsf{H}}$.

Further results concern the spectrum of the deflated matrix under the assumption of invariant deflation subspaces. The efficiency of deflation and augmentation methods in practice has been documented widely in the literature. Many of the references we give contain numerical examples of real-world problems.

Acknowledgments. The author is much indebted to André Gaul, Jörg Liesen, and Reinhard Nabben of the TU Berlin, not only for bringing up this topic and coauthoring with him the companion paper [28] on which sections 2 and 7 of the present paper build upon, but also for helping to reformulate and improve an earlier version of section 2. The author would also like to thank the referees as well as Yan-Fei Jing for carefully reading the paper, raising questions, and making suggestions for improvement.

REFERENCES

[1] A. M. Abdel-Rehim, R. B. Morgan, and W. Wilcox, *Deflated BiCGStab for linear equations in QCD problems*, preprint, arXiv:0710.1988, 2007.

[2] A. M. Abdel-Rehim, A. Stathopoulos, and K. Orginos, *Extending the eigCG Algorithm to Non-Symmetric Lanczos for Linear Systems with Multiple Right-Hand Sides*, Technical Report WM-CS-209-06, Department of Computer Science, College of William & Mary, Williamsburg, VA, 2009.

[3] K. Abe and G. L. Sleijpen, *BiCR variants of the hybrid BiCG methods for solving linear systems with nonsymmetric matrices*, J. Comput. Appl. Math., 234 (2009), pp. 985–994.

[4] K. Abe, T. Sogabe, S. Fujino, and S.-L. Zhang, *A product-type Krylov subspace method based on conjugate residual method for nonsymmetric coefficient matrices*, IPSJ Trans. Adv. Comput. Syst., 48 (2007), pp. 11–21 (in Japanese).

[5] K. Ahuja, *Recycling Bi-Lanczos Algorithms: BiCG, CGS, and BiCGSTAB*, Master Thesis etd-08252009-161256, Department of Mathematics, Virginia Polytechnic Institute and State University, 2009.

[6] K. Ahuja, E. de Sturler, S. Gugercin, and E. Chang, *Recycling BiCG with an application to model reduction*, SIAM J. Sci. Comput., 34 (2012), pp. A1925–A1949; see also arXiv: 1010.0762v4.

[7] J. I. Aliaga, D. L. Boley, R. W. Freund, and V. Hernández, *A Lanczos-type method for multiple starting vectors*, Math. Comp., 69 (2000), pp. 1577–1601.

[8] S. F. Ashby, T. A. Manteuffel, and P. E. Saylor, *A taxonomy for conjugate gradient methods*, SIAM J. Numer. Anal., 27 (1990), pp. 1542–1568.

[9] C. Beattie, S. Gugercin, and S. Wyatt, *Inexact solves in interpolatory model reduction*, Linear Algebra Appl., 436 (2012), pp. 2916–2943.

[10] P. N. Brown and H. F. Walker, *GMRES on (nearly) singular systems*, SIAM J. Matrix Anal. Appl., 18 (1997), pp. 37–51.

[11] E. de Sturler, *Nested Krylov methods based on GCR*, J. Comput. Appl. Math., 67 (1996), pp. 15–41.

[12] E. de Sturler, *Truncation strategies for optimal Krylov subspace methods*, SIAM J. Numer. Anal., 36 (1999), pp. 864–889.

[13] Z. Dostál, *Conjugate gradient method with preconditioning by projector*, Int. J. Comput. Math., 23 (1988), pp. 315–323.

[14] M. Eiermann, O. G. Ernst, and O. Schneider, *Analysis of acceleration strategies for restarted minimal residual methods*, J. Comput. Appl. Math., 123 (2000), pp. 261–292.

[15] S. C. Eisenstat, H. C. Elman, and M. H. Schultz, *Variational iterative methods for nonsymmetric systems of linear equations*, SIAM J. Numer. Anal., 20 (1983), pp. 345–357.

[16] J. Erhel and F. Guyomarc'h, *An augmented conjugate gradient method for solving consecutive symmetric positive definite linear systems*, SIAM J. Matrix Anal. Appl., 21 (2000), pp. 1279–1299.

[17] Y. A. Erlangga and R. Nabben, *Deflation and balancing preconditioners for Krylov subspace methods applied to nonsymmetric matrices*, SIAM J. Matrix Anal. Appl., 30 (2008), pp. 684–699.

[18] Y. A. Erlangga and R. Nabben, *On a multilevel Krylov method for the Helmholtz equation preconditioned by shifted Laplacian*, Electron. Trans. Numer. Anal., 31 (2008), pp. 403–424.

[19] Y. A. Erlangga and R. Nabben, *Algebraic multilevel Krylov methods*, SIAM J. Sci. Comput., 31 (2009), pp. 3417–3437.
[20] R. Fletcher, *Conjugate gradient methods for indefinite systems*, in Numerical Analysis, Dundee, 1975, G. A. Watson, ed., Lecture Notes in Math. 506, Springer, Berlin, 1976, pp. 73–89.
[21] J. Frank and C. Vuik, *On the construction of deflation-based preconditioners*, SIAM J. Sci. Comput., 23 (2001), pp. 442–462.
[22] R. W. Freund, *Band Lanczos method (section* 4.6*)*, in Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide, Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst, eds., SIAM, Philadelphia, 2000, pp. 80–88.
[23] R. W. Freund, *Band Lanczos method (section* 7.10*)*, in Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide, Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst, eds., SIAM, Philadelphia, 2000, pp. 205–216.
[24] R. W. Freund, M. H. Gutknecht, and N. M. Nachtigal, *An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices*, SIAM J. Sci. Comput., 14 (1993), pp. 137–158.
[25] R. W. Freund and M. Hochbruck, *On the use of two QMR algorithms for solving singular systems and applications in Markov chain modeling*, Numer. Linear Algebra Appl., 1 (1994), pp. 403–420.
[26] A. Gaul, *Recycling Krylov Subspace Methods for Sequences of Linear Systems. Analysis and Applications*, Ph.D. thesis, Technical University Berlin, 2014.
[27] A. Gaul, M. H. Gutknecht, J. Liesen, and R. Nabben, *Deflated and Augmented Krylov Subspace Methods: Basic Facts and a Breakdown-Free Deflated MINRES*, MATHEON Preprint 759, Technical University Berlin, 2011.
[28] A. Gaul, M. H. Gutknecht, J. Liesen, and R. Nabben, *A framework for deflated and augmented Krylov subspace methods*, SIAM J. Matrix Anal. Appl., 34 (2013), pp. 495–518; revised version of [27].
[29] M. H. Gutknecht, *The unsymmetric Lanczos algorithms and their relations to Padé approximation, continued fractions, and the QD algorithm*, in Preliminary Proceedings of the Copper Mountain Conference on Iterative Methods, 1990; http://www.sam.math.ethz.ch/~mhg/pub/CopperMtn90.ps.gz and http://www.sam.math.ethz.ch/~mhg/pub/CopperMtn90-7.ps.gz.
[30] M. H. Gutknecht, *Lanczos-type solvers for nonsymmetric linear systems of equations*, Acta Numer., 6 (1997), pp. 271–397.
[31] M. H. Gutknecht, *IDR explained*, Electron. Trans. Numer. Anal., 36 (2010), pp. 126–148.
[32] M. H. Gutknecht, *Spectral deflation in Krylov solvers: A theory of coordinate space based methods*, Electron. Trans. Numer. Anal., 39 (2012), pp. 156–185.
[33] Y.-F. Jing, T.-Z. Huang, Y. Zhang, L. Li, G.-H. Cheng, Z.-G. Ren, Y. Duan, T. Sogabe, and B. Carpentieri, *Lanczos-type variants of the COCR method for complex nonsymmetric linear systems*, J. Comput. Phys., 228 (2009), pp. 6376–6394.
[34] M. E. Kilmer and E. de Sturler, *Recycling subspace information for diffuse optical tomography*, SIAM J. Sci. Comput., 27 (2006), pp. 2140–2166.
[35] C. Lanczos, *Solution of systems of linear equations by minimized iterations*, J. Research Nat. Bur. Standards, 49 (1952), pp. 33–53.
[36] D. Loher, *Reliable Nonsymmetric Block Lanczos Algorithms*, Ph.D. thesis, Dissertation 16337, ETH Zurich, Zurich, Switzerland, 2006.
[37] R. B. Morgan, *A restarted GMRES method augmented with eigenvectors*, SIAM J. Matrix Anal. Appl., 16 (1995), pp. 1154–1171.
[38] R. B. Morgan, *GMRES with deflated restarting*, SIAM J. Sci. Comput., 24 (2002), pp. 20–37.
[39] R. Nabben and C. Vuik, *A comparison of deflation and coarse grid correction applied to porous media flow*, SIAM J. Numer. Anal., 42 (2004), pp. 1631–1647.
[40] R. Nabben and C. Vuik, *A comparison of deflation and the balancing preconditioner*, SIAM J. Sci. Comput., 27 (2006), pp. 1742–1759.
[41] R. Nabben and C. Vuik, *A comparison of abstract versions of deflation, balancing and additive coarse grid correction preconditioners*, Numer. Linear Algebra Appl., 15 (2008), pp. 355–372.
[42] R. A. Nicolaides, *Deflation of conjugate gradients with applications to boundary value problems*, SIAM J. Numer. Anal., 24 (1987), pp. 355–365.
[43] D. P. O'Leary, *The block conjugate gradient algorithm and related methods*, Linear Algebra Appl., 29 (1980), pp. 293–322.
[44] M. L. Parks, E. de Sturler, G. Mackey, D. D. Johnson, and S. Maiti, *Recycling Krylov subspaces for sequences of linear systems*, SIAM J. Sci. Comput., 28 (2006), pp. 1651–1674.

[45] A. Ruhe, *Implementation aspects of band Lanczos algorithms for computation of eigenvalues of large sparse symmetric matrices*, Math. Comp., 33 (1979), pp. 680–687.
[46] Y. Saad, *Analysis of augmented Krylov subspace methods*, SIAM J. Matrix Anal. Appl., 18 (1997), pp. 435–449.
[47] Y. Saad, M. Yeung, J. Erhel, and F. Guyomarc'h, *A deflated version of the conjugate gradient algorithm*, SIAM J. Sci. Comput., 21 (2000), pp. 1909–1926.
[48] V. Simoncini and D. B. Szyld, *Recent computational developments in Krylov subspace methods for linear systems*, Numer. Linear Algebra Appl., 14 (2007), pp. 1–59.
[49] V. Simoncini and D. B. Szyld, *Interpreting IDR as a Petrov–Galerkin method*, SIAM J. Sci. Comput., 32 (2010), pp. 1898–1912.
[50] T. Sogabe, *Extensions of the Conjugate Residual Method*, Ph.D. thesis, University of Tokyo, 2006.
[51] T. Sogabe, M. Sugihara, and S.-L. Zhang, *An extension of the conjugate residual method to nonsymmetric linear systems*, J. Comput. Appl. Math., 226 (2009), pp. 103–113.
[52] P. Sonneveld, *CGS, a fast Lanczos-type solver for nonsymmetric linear systems*, SIAM J. Sci. Statist. Comput., 10 (1989), pp. 36–52.
[53] P. Sonneveld and M. B. van Gijzen, IDR(s)*: A family of simple and fast algorithms for solving large nonsymmetric systems of linear equations*, SIAM J. Sci. Comput., 31 (2008), pp. 1035–1062.
[54] J. M. Tang, R. Nabben, C. Vuik, and Y. A. Erlangga, *Comparison of two-level preconditioners derived from deflation, domain decomposition and multigrid methods*, J. Sci. Comput., 39 (2009), pp. 340–370.
[55] H. A. van der Vorst, *Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems*, SIAM J. Sci. Statist. Comput., 13 (1992), pp. 631–644.
[56] M. B. van Gijzen and P. Sonneveld, *Algorithm* 913: *An elegant* IDR(s) *variant that efficiently exploits biorthogonality properties*, ACM Trans. Math. Software, 38 (2011), 5.
[57] S. Wang, E. de Sturler, and G. H. Paulino, *Large-scale topology optimization using preconditioned Krylov subspace methods with recycling*, Internat. J. Numer. Methods Engrg., 69 (2007), pp. 2441–2468.
[58] P. Wesseling and P. Sonneveld, *Numerical experiments with a multiple grid and a preconditioned Lanczos type method*, in Approximation Methods for Navier-Stokes Problems (Proc. Sympos., Univ. Paderborn, Paderborn, 1979), Lecture Notes in Math. 771, Springer, Berlin, 1980, pp. 543–562.
[59] M.-C. Yeung, *ML(n)BiCGStab: Reformulation, Analysis, and Implementation*, Report 09-01, Math. Dept., University of Wyoming; arXiv:1011.5314, 2010.
[60] M.-C. Yeung, *An Introduction to ML(n)BiCGStab*, Report 11-06, Math. Dept., University of Wyoming; arXiv:1106.3678, 2011.
[61] M.-C. Yeung and T. F. Chan, *ML(k)BiCGSTAB: A BiCGSTAB variant based on multiple Lanczos starting vectors*, SIAM J. Sci. Comput., 21 (1999), pp. 1263–1290.
[62] M. C. Yeung, J. M. Tang, and C. Vuik, *On the Convergence of GMRES with Invariant-Subspace Deflation*, Report 10-14, Delft Institute of Applied Mathematics, Delft University of Technology, 2010.
[63] D. M. Young and K. C. Jea, *Generalized conjugate-gradient acceleration of nonsymmetrizable iterative methods*, Linear Algebra Appl., 34 (1980), pp. 159–194.
[64] J. Zhang and J. Zhao, *A new variant of BiCRSTAB method for solving nonsymmetric indefinite linear systems*, J. Inform. Comput. Sci., 8 (2011), pp. 2183–2195.