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SPECTRAL DEFLATION IN KRYLOV SOLVERS: A THEORY OF COORDINATE SPACE BASED METHODS*

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Abstract. For the iterative solution of large sparse linear systems we develop a theory for a family of augmented and deflated Krylov space solvers that are coordinate based in the sense that the given problem is transformed into one that is formulated in terms of the coordinates with respect to the augmented bases of the Krylov subspaces. Except for the augmentation, the basis is as usual generated by an Arnoldi or Lanczos process, but now with a deflated, singular matrix. The idea behind deflation is to explicitly annihilate certain eigenvalues of the system matrix, typically eigenvalues of small absolute value. The deflation of the matrix is based on an either orthogonal or oblique projection on a subspace that is complimentary to the deflated approximately invariant subspace. While an orthogonal projection allows us to find minimal residual norm solutions, the oblique projections, which we favor when the matrix is non-Hermitian, allow us in the case of an exactly invariant subspace to correctly deflate both the right and the corresponding left (possibly generalized) eigenspaces of the matrix, so that convergence only depends on the non-deflated eigenspaces. The minimality of the residual is replaced by the minimality of a quasi-residual. Among the methods that we treat are primarily deflated versions of GMRES, MINRES, and QMR, but we also extend our approach to deflated, coordinate space based versions of other Krylov space methods including variants of CG and BICG. Numerical results will be published elsewhere.

Key words. Linear equations, Krylov space method, Krylov subspace method, deflation, augmented basis, recycling Krylov subspaces, (singular) preconditioning, GMRES, MINRES, QMR, CG, BICG

1. Introduction.

Krylov space solvers are the standard tool for solving very large sparse linear systems $\mathbf{Ax} = \mathbf{b}$ by iteration. But for many real-world problems they only converge in a reasonable number of iterations if a suitable preconditioning technique is applied. This is particularly true for problems where the matrix $\mathbf{A}$ has eigenvalues of small absolute value — a situation that is very common in practice. A complementary technique for dealing with such problems can be viewed as applying a singular left preconditioner that deflates the matrix in the sense that small eigenvalues are replaced by zero eigenvalues. We first have to identify an approximately invariant subspace $\mathcal{Z}$ that belongs to a set of such small eigenvalues. Ways to do that have been extensively discussed in the literature and will therefore not be a topic of this paper; see, *e.g.*, [1, 3, 6, 9, 12, 37, 42, 43, 44, 45, 48, 57, 62]. By using an orthogonal projection $\mathbf{P}$ whose nullspace is $\mathcal{Z}$ the Krylov space solver is then applied only to the orthogonal complement $\mathcal{Z}^\perp$ by restricting the operator $\mathbf{A}$ accordingly. The basis constructed implicitly or explicitly by this restricted operator is augmented by a set of basis vectors for $\mathcal{Z}$. In some algorithms based on short recurrences $\mathcal{Z}$ may also include eigenvectors that the iteration has identified well already and which in the sequel might cause loss of orthogonality if new basis vectors were not reorthogonalized against them. In practice, the dimension of the deflation space $\mathcal{Z}$ may get increased during the solution process or the space may get adapted, in particular if a restarted algorithm is employed. In this paper we assume for simplicity that $\mathcal{Z}$ is fixed.

A relevant detail of the approach discussed here is that the basis of $\mathcal{Z}$ is assumed to be given as the columns of a matrix of the form $\mathbf{Z} = \mathbf{AU}$. So, the preimage of the basis, the columns of $\mathbf{U}$, are assumed to be known. In practice this means that we choose first the matrix $\mathbf{U}$, which also spans an approximately invariant subspace $\mathcal{U}$ for the chosen eigenvalues, and then compute the image $\mathbf{Z} = \mathbf{AU}$. This implies that the restriction $\mathbf{A}|_{\mathcal{Z}}$ of $\mathbf{A}$ to $\mathcal{Z}$ can be

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inverted trivially: if, say, $\mathbf{y} = \mathbf{Zk} \in \mathcal{Z}$, then $\mathbf{A}^{-1}\mathbf{y} = \mathbf{A}^{-1}\mathbf{Zk} = \mathbf{Uk} \in \mathcal{U}$.

Applying a Krylov space solver to a linear system $\mathbf{Ax} = \mathbf{b}$ means to construct a sequence of approximate solutions $\mathbf{x}_n$ that are of the form $\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$, where $\mathbf{x}_0$ is a chosen initial approximation, $\mathbf{r}_0 :\equiv \mathbf{b} - \mathbf{Ax}_0$ is the corresponding residual, and $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ is the nth Krylov subspace generated by $\mathbf{A}$ from $\mathbf{r}_0$. (For its definition see Section 2.) Then, $\mathbf{r}_n \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$, and the goal is to make $\mathbf{r}_n$ small in some norm. Therefore, solving the linear system with a Krylov space solver can be understood as successively approximating $\mathbf{r}_0$ by elements of the subspaces $\mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$.

In the methods described here first, $\mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ will be replaced by the subspace $\mathbf{A}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$, where the deflated operator $\widehat{\mathbf{A}} :\equiv \mathbf{PAP}$ is singular, and $\widehat{\mathbf{r}}_0 :\equiv \mathbf{Pr}_0 \in \mathcal{Z}^\perp$, so that we will have $\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) \subseteq \mathcal{Z}^\perp$. Note that on $\mathcal{Z}^\perp$, and thus also on the Krylov subspace, the restriction of $\widehat{\mathbf{A}}$ is equal to the restriction of $\mathbf{PA}$; thus only one application of $\mathbf{P}$ is needed for applying $\widehat{\mathbf{A}}$. On the other hand, as search space for approximate solutions $\mathbf{x}_n$, this Krylov subspace will be augmented by $\mathcal{U}$, that is,

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{U}\,, \qquad \mathbf{r}_n \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) + \mathcal{Z}\,. \tag{1.1}$$

If $\mathcal{Z}^\perp$ is $\mathbf{A}$-invariant, $\mathbf{A}\mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) \subseteq \mathcal{Z}^\perp$, so we can view the approach chosen here as splitting up $\mathbf{r}_0$ in its two orthogonal components $\widehat{\mathbf{r}}_0 \in \mathcal{Z}^\perp$ and $\mathbf{r}_0 - \widehat{\mathbf{r}}_0 \in \mathcal{Z}$. The preimage of the latter component can be computed in the trivial way outlined before, while the preimage of $\widehat{\mathbf{r}}_0$ is approximately computed with a Krylov space solver for $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ acting only in $\mathcal{Z}^\perp$. However, some complications occur if $\mathcal{Z}^\perp$ is not $\mathbf{A}$-invariant, which is the usual case. Treating these complications suitably is the main aim of this paper. In any case, we will see that we can first solve the restricted problem $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ by a standard method such as GMRES [53] and subsequently compute the still 'missing' component of the solution by solving a small triangular linear system.

While we will quickly also review the 'symmetric case', where the linear system is Hermitian (or real and symmetric), we are here mostly interested in the 'non-symmetric case', where our main message is that it may be preferable to replace the orthogonal decomposition of $\mathbf{r}_0$ by a non-orthogonal one. To this end, $\mathbf{P}$ must be chosen as an oblique projection with the property that when its nullspace $\mathcal{Z}$ is $\mathbf{A}$–invariant, so is its range $\widetilde{\mathcal{Z}}^\perp$. In this way, we not only can annul eigenvalues, but also deflate the corresponding left and right invariant subspaces. This choice leads then in a straightforward way to a 'truly deflated' GMRES and to deflated QMR [28]. Like in the symmetric case, if $\mathcal{Z}$ is $\mathbf{A}$–invariant, the convergence speed of the deflated method is then fully determined by the nondeflated eigenvalues of $\mathbf{A}$ and the corresponding invariant subspace. There is no need for deriving new convergence estimates unless we want to estimate the influence of an inexact choice of the subspace.

Our general approach can be used to define deflated versions of any Krylov space solver. But in this paper we concentrate on coordinate space based methods such as GMRES, MINRES [49], and QMR, where the Arnoldi or the Lanczos method is used to generate a series of bases of the nested Krylov subspaces. As is well known, this allows us to reformulate a minimum residual problem as an equivalent or approximately equivalent least squares problem in coordinate space, which can be solved by updating the QR decomposition of a Hessenberg or tridiagonal matrix.

Orthogonal and biorthogonal residual methods such as CG [34] and BICG [40, 23] can also be realized in this way, but are then normally considered less attractive, perhaps due to the possible nonexistence of some of the iterates. Here, at the end, we only introduce related deflated quasi-(bi)orthogonal residual methods.

A further main goal of this paper is to present all these methods in a common framework that relies on a splitting of the space into two complementary subspaces, which can be chosen in various ways. We favor here the above mentioned choice reflecting a partition of the spectrum, but in the nonsymmetric case this leads to a conflict with the choice imposed by residual minimization. In contrast to our treatment, the excellent general treatment and review of augmentation methods by Eiermann, Ernst, and Schneider [16] is mostly restricted to the application of orthogonal projections and does not capitalize upon the knowledge of bases for both $\mathcal{U}$ and $\mathcal{Z}$ assumed here (unless they are $\mathbf{A}$–invariant and thus equal). A further difference is that their treatment is aiming for augmented minimal residual methods, in particular GMRES, while we will drop optimality in Sections 5–9 and replace it by some near-optimality. Another interesting discussion and review of augmentation and deflation methods is due to Simoncini and Szyld [55, §9].

It is a well-known fact about Krylov space solvers that aiming for the smallest 2-norm of the residual, that is, applying GMRES without restarts, is not only excessively memory consuming, but is often also not much faster than using alternative methods that are suboptimal. In practice, it is not important to find the fastest solver, but to apply an effective preconditioning or multilevel method. Augmentation and deflation are powerful options along these lines, and there are several different ways to apply the basic ideas. Moreover, it is no problem to combine them with other preconditioning techniques.

Literature. Augmentation and deflation of Krylov space solvers have been proposed in various forms in a large number of publications. Many of the methods differ not only algorithmically and numerically, but also mathematically. Some keywords associated with such methods are '(spectral) deflation', 'augmented bases', 'recycling Krylov subspaces', 'spectral preconditioning', and 'singular preconditioning'. The primary goal is always to speed up the convergence of a solver, but the application to linear systems with multiple right-hand sides and to systems with slowly changing matrix and right-hand side is also often mentioned.

To our knowledge, the first suggestion of an augmented Krylov space method that included both the deflation of the matrix and the corresponding projection of the initial residual came from Nicolaides [48], who submitted on May 13, 1985, such a deflated CG algorithms based on the three-term recursions for iterates and residuals. Independently, Dostál [13] submitted in January 1987 a mathematically equivalent deflated CG algorithm based on the well-known coupled two-term recursions; he even gave an estimate for the improvement of the condition number. In June 1987 Mansfield [41] submitted additional numerical evidence for what he referred to as Nicolaides' method of deflation, but he was actually using a 2-term CG algorithm. The same algorithm was more than ten years later again discovered by Erhel and Guyomarc'h [19] (deflation of a previously constructed Krylov subspace), by Saad, Yeung, Erhel, and Guyomarc'h [54], and, independently, by Vuik, Segal, and Meijerink [61], who combined it with preconditioning by incomplete Cholesky decomposition. All three papers refer to Nicolaides [48], but not to Dostál [13] and Mansfield [41], whose articles are much closer to their work. From a Google scholar search one can conclude that it was Kolotilina [39] who ultimately promoted Dostál's paper [13] to a larger audience. But, his two related papers [14, 15] are not even mentioned by her. Early citations to Mansfield, who also had two follow up papers, are by Fischer [22] and Kolotilina [39]. To achieve the optimality of the CG error vector in the $\mathbf{A}$-norm an oblique projection has to be used (see Sections 11 and 12), which can be viewed as an $\mathbf{A}$-orthogonal projection however, and has nothing to do with the oblique projections promoted here. Before, in 1992, Kharchenko and Yeremin [37], followed, in 1994, by Erhel, Burrage, and Pohl [18] suggested GMRES algorithms with augmented basis and a corresponding nonsingular right preconditioner that moves the small eigenvalues to a multiple large eigenvalue. Later Baglama, Calvetti, Golub, and Reichel [6] constructed a left preconditioner with the same effect; see [16, pp. 286–289] for a brief comparison of these three preconditioners. Also in the mid-1990s, Morgan [43] proposed GMRES with augmented basis but no explicit deflation of the matrix, and de Sturler [11] suggested an inner-outer GMRES/GCR algorithm with augmented basis and later, in other publications, several related methods. Saad [52] put together a general analysis of Krylov space methods with augmented basis, which was further generalized in the above mentioned survey article of Eiermann, Ernst, and Schneider [16]. Many more publications followed; see, *e.g.*, [1, 24, 45, 57, 63] for further references. The starting point for the present paper has been the description of recycled MINRES or RMINRES by Wang, de Sturler, and Paulino [62], which, after a minor modification that does not change the mathematical properties, fits exactly into our framework. Their orthogonal projection $\mathbf{P}$ and the corresponding deflated matrix $\widehat{\mathbf{A}}$ have been used before, *e.g.*, in [16, 11, 12]. They are the basic tools of our approach in 2–4. But so far the oblique projection $\mathbf{P}$ that is the basis of our approaches of Sections 5–9 only seems to have been used for Ahuja's Recycling BICG(RBICG) [4, 5], which does not fit into our framework; see Section 12 for how it relates to our work. In particular, the oblique projection applied by Erlangga and Nabben [20] for their version of deflated GMRES is different from our. In fact, the projection of [20] generalizes the one that is typical for deflated CG [48, 13, 41]. The connection to some of these alternative choices will be explained in Section 11. Our approach is also different from the one of Abdel-Rehim, Morgan, and Wilcox [2] for their deflated BICGSTAB, and the one of Abdel-Rehim, Stathopoulos, and Orginos [3] for their Lanczos based combined equation and eigenvalue solver.

We must also mention that in a series of papers that culminates in [21, 47, 60] it has been shown recently that deflation, domain decomposition, and multigrid can be viewed as instances of a common algebraic framework.

Outline. We start in Section 2 by introducing the basic setting for a particular version of augmented and deflated GMRES based on an orthogonal projection that annuls approximate small eigenvalues, in the sense that they get moved to zero. The possibility of breakdowns of this method and its adaptation to symmetric problems, where GMRES turns into MINRES, are then discussed in Sections 3–4. In Sections 5–6, we modify the basic setting by introducing an oblique projection that enables us to deflate approximate (possibly generalized) eigenspaces and to introduce a truly deflated GMRES method. By making use of an adjoint Krylov space generated by $\widehat{\mathbf{A}}^{\mathsf{H}}$ we next explain in Sections 7–9 how we can adapt our approach to the nonsymmetric Lanczos algorithm and introduce a deflated QMR method and a simplified deflated QMR method. The latter has, *e.g.*, a well-known application in quantum chromodynamics. Moreover, in Section 10 we describe a different way of computing the component of the solution that lies in $\mathcal{U}$, and in Section 12 we briefly point out that our framework could in principle also be used to define coordinate space based deflated (bi)orthogonal residual methods that are approximately equivalent to deflated CG and BICG methods.

Notation. We denote the range (or, the image) of a matrix $\mathbf{M}$ by $\mathcal{R}(\mathbf{M})$. For the nullspace (or kernel) of $\mathbf{M}$ we write $\mathcal{N}(\mathbf{M})$. Sometimes we introduce the additional notation $\mathcal{M} :\equiv \mathcal{R}(\mathbf{M})$ for the range. As usual, the first column of the $n \times n$ unit matrix is $\mathbf{e}_1$; additionally, $\underline{\mathbf{e}}_1 \in \mathbb{R}^{n+1}$ is $\mathbf{e}_1$ with a extra zero component appended to it. Likewise, $\underline{\mathbf{H}}_n$ and $\underline{\mathbf{T}}_n$ will be $(n+1) \times n$ matrices whose top $n \times n$ submatrices are $\mathbf{H}_n$ and $\mathbf{T}_n$, respectively.

2. Deflation by orthogonal projection; deflated GMRES. Consider a nonsingular linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ of size $N \times N$. Let $\mathbf{U} \in \mathbb{C}^{N \times k}$ have full rank k, where $1 \le k < N$, and set

$$\mathcal{U} :\equiv \mathcal{R}(\mathbf{U}), \qquad \mathbf{Z} :\equiv \mathbf{A}\mathbf{U}, \qquad \mathcal{Z} :\equiv \mathcal{R}(\mathbf{Z}) = \mathbf{A}\mathcal{U},$$

and

$$\mathbf{E} :\equiv \mathbf{Z}^{\mathsf{H}}\mathbf{Z}, \qquad \mathbf{Q} :\equiv \mathbf{Z}\mathbf{E}^{-1}\mathbf{Z}^{\mathsf{H}}, \qquad \mathbf{P} :\equiv \mathbf{I} - \mathbf{Q} = \mathbf{I} - \mathbf{Z}\mathbf{E}^{-1}\mathbf{Z}^{\mathsf{H}}.$$

The subspaces $\mathcal{U}$ and $\mathcal{Z}$ will be used to augment the search spaces for the approximate solutions $\mathbf{x}_n$ and the corresponding residuals $\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{A}\mathbf{x}_n$, respectively. Note that $\mathbf{Q}^2 = \mathbf{Q}$, $\mathbf{P}^2 = \mathbf{P}$, $\mathbf{Q}^{\mathsf{H}} = \mathbf{Q}$, and $\mathbf{P}^{\mathsf{H}} = \mathbf{P}$; so, $\mathbf{Q}$ is the orthogonal projection onto $\mathcal{Z}$, while $\mathbf{P}$ is the orthogonal projection onto the orthogonal complement $\mathcal{Z}^\perp$ of $\mathcal{Z}$.

If the columns $\mathbf{u}_j$ of $\mathbf{U} \in \mathbb{C}^{N\times k}$ are chosen to be $\mathbf{A}^{\mathsf{H}}\mathbf{A}$-orthonormal, so that the columns of $\mathbf{Z} = \mathbf{A}\mathbf{U}$ form an orthonormal basis of $\mathcal{Z}$, which we will from now on assume, then $\mathbf{E} = \mathbf{I}_k$ and the formulas for $\mathbf{Q}$ and $\mathbf{P}$ simplify to

$$\mathbf{Q} = \mathbf{Z}\mathbf{Z}^{\mathsf{H}}\,, \qquad \mathbf{P} = \mathbf{I} - \mathbf{Q} = \mathbf{I} - \mathbf{Z}\mathbf{Z}^{\mathsf{H}}\,. \tag{2.1}$$

Alternatively, we could compute a QR decomposition of $\mathbf{A}\mathbf{U}$ to find a matrix $\mathbf{Z}$ with orthonormal columns; see Section 6, where we will temporarily apply this.

As mentioned in the introduction, the first basic idea is to restrict the Krylov space solver to $\mathcal{Z}^\perp$ by projecting the initial residual $\mathbf{r}_0$ into this space and by replacing the original operator $\mathbf{A}$ by its restriction to this space:

$$\widehat{\mathbf{r}}_0 :\equiv \mathbf{P}\mathbf{r}_0\,, \qquad \widehat{\mathbf{A}} :\equiv \mathbf{P}\mathbf{A}\mathbf{P}\,.$$

A corresponding initial approximation $\widehat{\mathbf{x}}_0$ is not needed. (Any $\widehat{\mathbf{x}}_0 \in \mathbf{x}_0 + \mathcal{U}$ would satisfy $\widehat{\mathbf{r}}_0 :\equiv \mathbf{P}\mathbf{r}_0 = \mathbf{P}(\mathbf{b} - \mathbf{A}\mathbf{x}_0) = \mathbf{P}(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_0)$, and for theoretical purposes we could even set $\widehat{\mathbf{x}}_0 :\equiv \mathbf{A}^{-1}\mathbf{P}\mathbf{A}\mathbf{x}_0$ to achieve that $\widehat{\mathbf{r}}_0 = \mathbf{P}\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_0$, or $\widehat{\mathbf{x}}_0 :\equiv \mathbf{A}^{-1}(\mathbf{P}\mathbf{A}\mathbf{x}_0 + \mathbf{Q}\mathbf{b})$ to achieve that $\widehat{\mathbf{r}}_0 = \mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_0$.) Note that $\operatorname{rank}\widehat{\mathbf{A}} \le N - k$ since $\operatorname{rank}\mathbf{P} = N - k$, so $\widehat{\mathbf{A}}$ is always singular.

Given any initial guess $\mathbf{x}_0$, the second basic idea is to approximate the solution $\mathbf{x}_\star :\equiv \mathbf{A}^{-1}\mathbf{b}$ by iterates $\mathbf{x}_n$ from the following affine space:

$$\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}\,, \tag{2.2}$$

where

$$\widehat{\mathcal{K}}_n :\equiv \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0) :\equiv \operatorname{span}\{\widehat{\mathbf{r}}_0, \widehat{\mathbf{A}}\widehat{\mathbf{r}}_0, \ldots, \widehat{\mathbf{A}}^{n-1}\widehat{\mathbf{r}}_0\} \tag{2.3}$$

is the nth Krylov subspace generated by $\widehat{\mathbf{A}}$ from $\widehat{\mathbf{r}}_0$. Since $\widehat{\mathbf{r}}_0 \in \mathcal{Z}^\perp$ and $\mathcal{R}(\widehat{\mathbf{A}}) \subseteq \mathcal{R}(\mathbf{P}) = \mathcal{Z}^\perp$, we have $\widehat{\mathcal{K}}_n \subseteq \mathcal{Z}^\perp$. The choice (2.2) implies that

$$\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{A}\mathbf{x}_n \in \mathbf{r}_0 + \mathbf{A}\widehat{\mathcal{K}}_n + \mathcal{Z}\,. \tag{2.4}$$

If we construct a nested sequence of orthogonal bases for the Krylov subspaces $\widehat{\mathcal{K}}_n$ by an Arnoldi process started with $\mathbf{v}_0 :\equiv \widehat{\mathbf{r}}_0/\beta$, where $\beta :\equiv \|\widehat{\mathbf{r}}_0\|_2$, we can express this, for each n, by the Arnoldi relation $\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n$, with $\mathbf{V}_n :\equiv \begin{bmatrix} \mathbf{v}_0 & \ldots & \mathbf{v}_{n-1} \end{bmatrix}$ and an extended $(n+1)\times n$ upper Hessenberg matrix $\underline{\mathbf{H}}_n$. But since $\mathcal{R}(\mathbf{V}_n) = \widehat{\mathcal{K}}_n \subseteq \mathcal{Z}^\perp$, we have $\mathbf{P}\mathbf{V}_n = \mathbf{V}_n$, and therefore

$$\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{P}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{V}_n\,, \tag{2.5}$$

so that the Arnoldi relation simplifies to

$$\mathbf{P}\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n\,. \tag{2.6}$$

This means that only one projection $\mathbf{P}$ is needed for applying $\widehat{\mathbf{A}}$ in $\mathcal{Z}^\perp$.

In view of (2.2) we can represent $\mathbf{x}_n$ as

$$\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n + \mathbf{U}\mathbf{m}_n \tag{2.7}$$

with coordinate vectors $\mathbf{k}_n \in \mathbb{C}^n$ and $\mathbf{m}_n \in \mathbb{C}^k$. In the usual way, multiplication by $\mathbf{A}$ and subtraction from $\mathbf{b}$ yields then for the residuals $\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{A}\mathbf{x}_n$ the representation

$$\mathbf{r}_n = \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}\mathbf{m}_n \,. \tag{2.8}$$

Due to the Arnoldi relation (2.6) and the orthogonal decomposition $\mathbf{r}_0 = \widehat{\mathbf{r}}_0 + \mathbf{Q}\mathbf{r}_0 = \mathbf{v}_0\beta + \mathbf{Q}\mathbf{r}_0$ this becomes, with $\mathbf{C}_n :\equiv \mathbf{Z}^{\mathsf{H}}\mathbf{A}\mathbf{V}_n \in \mathbb{C}^{k\times n}$ and $\mathbf{Q} = \mathbf{Z}\mathbf{Z}^{\mathsf{H}}$, and in analogy to the derivation for the symmetric case in [62][1],

$$\begin{aligned}\mathbf{r}_n &= \mathbf{v}_0\beta + \mathbf{Q}\mathbf{r}_0 - (\mathbf{P}+\mathbf{Q})\mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}\mathbf{m}_n \\ &= \begin{bmatrix} \mathbf{Z} & \mathbf{V}_{n+1} \end{bmatrix} \underline{\mathbf{q}}_n \,,\end{aligned} \tag{2.9}$$

where

$$\underline{\mathbf{q}}_n :\equiv \begin{bmatrix} \mathbf{Z}^{\mathsf{H}}\mathbf{r}_0 \\ \underline{\mathbf{e}}_1\beta \end{bmatrix} - \begin{bmatrix} \mathbf{I}_k & \mathbf{C}_n \\ \mathbf{O} & \underline{\mathbf{H}}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} \quad \in \mathbb{C}^{k+n+1} \tag{2.10}$$

may be called *deflated* GMRES *quasi-residual* in analogy to the terminology of [28]. One option is to choose $\mathbf{r}_n$ of minimal 2-norm. Then (2.9) is the key relation for a GMRES-like approach to this problem: $\mathbf{r}_n$ is represented in terms of the basis consisting of the columns of $\mathbf{Z}$ and $\mathbf{V}_{n+1}$. Since we assume $\mathbf{Z}$ to have orthonormal columns as in (2.1), $\begin{bmatrix} \mathbf{Z} & \mathbf{V}_{n+1} \end{bmatrix}$ has orthonormal columns too, and the coordinate map is isometric in the 2-norms of $\mathcal{Z} \oplus \mathcal{R}(\mathbf{V}_{n+1}) \subseteq \mathbb{C}^N$ and $\mathbb{C}^{k+n+1}$, respectively, so that

$$\|\mathbf{r}_n\|_2 = \|\underline{\mathbf{q}}_n\|_2 = \left\| \begin{bmatrix} \mathbf{Z}^{\mathsf{H}}\mathbf{r}_0 \\ \underline{\mathbf{e}}_1\beta \end{bmatrix} - \begin{bmatrix} \mathbf{I}_k & \mathbf{C}_n \\ \mathbf{O} & \underline{\mathbf{H}}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} \right\|_2 . \tag{2.11}$$

As in the original GMRES method [53] the minimization of $\|\mathbf{r}_n\|_2$ reduces in the nth step to a least squares problem for minimizing the right-hand side of (2.11), which can be solved recursively by updating in each iteration the QR decomposition of the $(n+1)\times n$ Hessenberg matrix $\underline{\mathbf{H}}_n$. Note that the first k columns of the least square problem are in diagonal form, hence, *a fortiori* in upper triangular form already. Hence, the $(k+n+1)\times(k+n)$ least squares problem in (2.11) decouples from the beginning into an $(n+1)\times n$ least squares problem for $\mathbf{k}_n$ and an explicit formula for $\mathbf{m}_n$:

$$\min \|\mathbf{r}_n\|_2 = \min \|\underline{\mathbf{q}}_n\|_2 = \min_{\mathbf{k}_n\in\mathbb{C}^n} \|\underline{\mathbf{e}}_1\beta - \underline{\mathbf{H}}_n\mathbf{k}_n\|_2 \,, \qquad \mathbf{m}_n := \mathbf{Z}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n \,. \tag{2.12}$$

This decomposition of the problem suggests that we search first for a solution of the reduced least squares problem, that is, determine a suitable size n, the matrices $\mathbf{V}_n$ and $\underline{\mathbf{H}}_n$ resulting from the Arnoldi process, and the corresponding solution $\mathbf{k}_n$ in coordinate space. This first stage can be understood as solving the singularly preconditioned system $\mathbf{PAx} = \mathbf{Pb}$ by standard GMRES, or as solving $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ in $\mathcal{Z}^\perp$ by GMRES. Subsequently, we may calculate the related $\mathbf{m}_n$. There is no need to compute $\mathbf{m}_n$ for all n since the 2-norm of the residual $\mathbf{r}_n$ is not affected by the second stage if $\mathbf{m}_n$ is chosen according to (2.12).

We will call the resulting algorithm *deflated* GMRES though it is not equivalent to the methods introduced by Morgan [43] and Chapman and Saad [9] under this name.[2] Our proposal also differs from those of Kharchenko and Yeremin [37] and Erhel, Burrage, and Pohl

[1] To change to the notation of [62] substitute, in particular, $\mathbf{Z} \rightsquigarrow \mathbf{C}$ and $\mathbf{C}_n \rightsquigarrow \mathbf{B}_n$.

[2] In both [9] and [43] a cycle of deflated GMRES consists in first applying a fixed number of GMRES steps with $\mathbf{A}$ starting from $\mathbf{x}_0$ (instead of using $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{x}}_0$), and then adding k orthogonalization steps to the vectors $\mathbf{A}\mathbf{u}_j$. This yields at the end an $(m+k+1)\times(m+k)$ least squares problem. So the orthogonal projection $\mathbf{P}$ is only applied at the end of each cycle. For an alternative interpretation and realization of Morgan's method see [16, §4.3] and [44].

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[18], who construct nonsingular preconditioners that move small eigenvalues away from zero. However, in Section 5 we will come up with another proposal for the nonsymmetric case, which we think is better suited to deflate approximate eigenpairs.

3. Breakdowns of deflated GMRES. Unfortunately, in general, the deflated GMRES method of Section 2 can break down since the Arnoldi process described by the relation $\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n$, which is used to set up the least squares problem in (2.12), is applied with a singular matrix $\widehat{\mathbf{A}}$. The least squares problem originates from solving $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ by GMRES for some $\widehat{\mathbf{x}} \in \mathcal{Z}^\perp$. Since $\mathcal{R}(\widehat{\mathbf{A}}) \subseteq \mathcal{Z}^\perp$ and $\widehat{\mathbf{r}}_0 \in \mathcal{Z}^\perp$, the linear system and the Arnoldi process are restricted to $\mathcal{Z}^\perp$. Hence, it is the restriction of $\widehat{\mathbf{A}}$ to $\mathcal{Z}^\perp$ which matters. This restriction is singular if and only if $\mathsf{rank}\,\widehat{\mathbf{A}} < N - k = \mathsf{dim}\,\mathcal{Z}^\perp$. But recall that in applications the eigenvalues of this restriction are supposed to approximate the nondeflated 'large' eigenvalues of $\mathbf{A}$; therefore, in practice it is very unlikely that the restriction is singular and breakdowns can occur.

If $\mathsf{rank}\,\widehat{\mathbf{A}} < N - k$, it may happen that $\mathbf{v}_0 \in \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp$ or that, for some $n > 1$, $\mathbf{v}_{n-1} \in \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{R}(\widehat{\mathbf{A}}) \subseteq \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp$. Then $\widehat{\mathbf{A}}\mathbf{v}_{n-1} = \mathbf{o}$ and, trivially, the component orthogonal to $\widehat{\mathcal{K}}_n = \mathcal{R}(\mathbf{V}_n)$ of this vector is also zero and cannot be normalized. Moreover, $\mathbf{V}_n^{\mathsf{H}}\widehat{\mathbf{A}}\mathbf{v}_{n-1} = \mathbf{V}_n^{\mathsf{H}}\mathbf{o} = \mathbf{o}$, so the last column of $\underline{\mathbf{H}}_n$ is zero except for its undetermined $(n+1, n)$–element, which we may set equal to 0 too. In particular, the top square part $\mathbf{H}_n$ of $\underline{\mathbf{H}}_n$ is singular. Hence, the Arnoldi process terminates after detecting the invariant subspace $\mathcal{R}(\mathbf{V}_n) = \widehat{\mathcal{K}}_n$, and GMRES breaks down. Note that $\mathsf{dim}\,(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = \mathsf{rank}\,(\widehat{\mathbf{A}}\mathbf{V}_n) = \mathsf{rank}\,(\mathbf{V}_n\mathbf{H}_n) = n - 1$ since $\mathsf{rank}\,\mathbf{H}_n = n - 1$. Is this the only type of breakdown?

The application of Krylov space methods to singular systems has been investigated in detail by Freund and Hochbruck [27, §§ 3-4] and others. In particular, the application of GMRES to such systems has been analyzed by Brown and Walker [8]. Lemma 2.1 of [8] adapted to our situation reads as follows.

LEMMA 1. *If* GMRES *is applied to* $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ *and if* $\dim \widehat{\mathcal{K}}_n = n$ *holds for some* $n \geq 1$, *then exactly one of the following three statements holds:*

(i) $\dim(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = n - 1$ *and* $\widehat{\mathbf{A}}\widehat{\mathbf{x}} \neq \widehat{\mathbf{r}}_0$ *for every* $\widehat{\mathbf{x}} \in \widehat{\mathcal{K}}_n$*;*

(ii) $\dim(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = \dim \widehat{\mathcal{K}}_{n+1} = n$, $\widehat{\mathbf{x}}_n :\equiv \mathbf{V}_n\mathbf{k}_n$ *is uniquely defined, and* $\widehat{\mathbf{A}}\widehat{\mathbf{x}}_n = \widehat{\mathbf{r}}_0$*;*

(iii) $\dim(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = n$, $\dim \widehat{\mathcal{K}}_{n+1} = n + 1$, $\widehat{\mathbf{x}}_n$ *is uniquely defined, but* $\widehat{\mathbf{A}}\widehat{\mathbf{x}}_n \neq \widehat{\mathbf{r}}_0$.

We call Case (i) a *breakdown* of GMRES, Case (ii) the *termination* of GMRES, and Case (iii) the *continuation* of GMRES. (In contrast, Brown and Walker [8] and other authors also call Case (ii) a breakdown, although in this case the aim of finding a solution of the linear system has been achieved.) Note that Case (i) implies that $\dim \widehat{\mathcal{K}}_{n+1} = n$, hence also in this case the Krylov space is exhausted.

In the situation where $\widehat{\mathbf{A}}\mathbf{v}_{n-1} = \mathbf{o}$ discussed before, we have obviously Case (i) since Arnoldi terminates, but the resulting equation $\underline{\mathbf{e}}_1\beta = \mathbf{H}_n\mathbf{k}_n$ has no solution. That this is more generally a consequence of $\dim(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = n - 1$ can be seen as follows: if we had chosen for $\widehat{\mathcal{K}}_n$ the so-called Krylov basis, that is

$$\mathbf{V}_n^{(\mathsf{K})} :\equiv \left[\begin{array}{cccc} \widehat{\mathbf{r}}_0 & \mathbf{A}\widehat{\mathbf{r}}_0 & \ldots & \mathbf{A}^{n-1}\widehat{\mathbf{r}}_0 \end{array}\right],$$

then, in Case (i), the Hessenberg relation resulting after n steps would be $\widehat{\mathbf{A}}\mathbf{V}_n^{(\mathsf{K})} = \mathbf{V}_n^{(\mathsf{K})}\mathbf{H}_n^{(\mathsf{K})}$, with a companion matrix $\mathbf{H}_n^{(\mathsf{K})}$ that has a zero element in its upper right corner, so that $\underline{\mathbf{e}}_1 \notin \mathcal{R}(\mathbf{H}_n^{(\mathsf{K})})$. This just reflects the fact that the restriction of $\widehat{\mathbf{A}}$ to $\widehat{\mathcal{K}}_n$ has a zero eigenvalue: the last column of $\mathbf{H}_n^{(\mathsf{K})}$ contains the coefficients of the characteristic polynomial. Note also that the basis transformation from $\mathbf{V}_n$ to $\mathbf{V}_n^{(\mathsf{K})}$ is represented by a triangular matrix and leaves the direction of the first basis vector invariant.

Clearly, $\dim(\widehat{\mathbf{A}}\widehat{\mathcal{K}}_n) = n-1$ (*i.e.*, Case (i)) holds if and only if $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$. Conversely, if this breakdown condition does not occur for any n, GMRES will ultimately terminate with Case (ii), where the unique solution of $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ is found. At intermediate steps, where Case (iii) occurs, $\widehat{\mathbf{x}}_n = \mathbf{V}_n \mathbf{k}_n$ is the best least squares solution out of $\widehat{\mathcal{K}}_n$.

In summary we obtain for deflated GMRES applied to $\mathbf{A}\mathbf{x} = \mathbf{b}$ the following theorem.

THEOREM 2. *If $\widehat{\mathbf{r}}_0 \notin \mathcal{N}(\widehat{\mathbf{A}})$, then as long as $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n = \{\mathbf{o}\}$, the deflated* GMRES *method defined by* (2.6)–(2.7) *and* (2.12) *yields in the nth step the approximate solution $\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ whose residual $\mathbf{r}_n$ has minimal 2-norm.*

However, if $\mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp \neq \{\mathbf{o}\}$ and if $\mathbf{x}_0$ is chosen such that $\widehat{\mathbf{r}}_0 \in \mathcal{N}(\widehat{\mathbf{A}})$, then (*and only then*) *deflated* GMRES *breaks down in the first step where $n = 1$. Moreover, at step $n > 1$, if* (*and only if*) *$\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$, the method breaks down when attempting to construct $\mathbf{v}_n$. In case of a breakdown, the search space $\mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ does not contain the exact solution $\mathbf{x}_\star$.*

If $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant, breakdowns cannot happen, $\mathbf{C}_n = \mathbf{O}$, and the Arnoldi relation (2.6) *can be replaced by*

$$\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n \,. \tag{3.1}$$

Proof. It remains to prove the last two sentences. Firstly, for a proof by contradiction, assume that the search space contains $\mathbf{x}_\star$, so $\mathbf{x}_\star :\equiv \mathbf{A}^{-1}\mathbf{b} = \mathbf{x}_0 + \widehat{\mathbf{x}}_\star + \mathbf{u}_\star$, where $\widehat{\mathbf{x}}_\star \in \widehat{\mathcal{K}}_n$ and $\mathbf{u}_\star \in \mathcal{U}$. Then, since $\mathbf{P}\mathbf{A}\mathbf{u}_\star = \mathbf{o}$ and $\mathbf{P}\mathbf{A}\widehat{\mathbf{x}}_\star = \widehat{\mathbf{A}}\widehat{\mathbf{x}}_\star$,

$$\begin{aligned}
\mathbf{o} &= \mathbf{b} - \mathbf{A}(\mathbf{x}_0 + \widehat{\mathbf{x}}_\star + \mathbf{u}_\star) \\
&= \mathbf{P}\mathbf{r}_0 - \mathbf{P}\mathbf{A}\widehat{\mathbf{x}}_\star - \mathbf{P}\mathbf{A}\mathbf{u}_\star + (\mathbf{I} - \mathbf{P})(\mathbf{r}_0 - \mathbf{A}\widehat{\mathbf{x}}_\star - \mathbf{A}\mathbf{u}_\star) \\
&= (\widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}\widehat{\mathbf{x}}_\star) + \mathbf{Q}(\mathbf{r}_0 - \mathbf{A}\widehat{\mathbf{x}}_\star - \mathbf{A}\mathbf{u}_\star)\,.
\end{aligned}$$

Since the first parenthesis is in $\mathcal{Z}^\perp$, while the second term is in $\mathcal{Z}$, both must be zero. In particular, we must have $\widehat{\mathbf{r}}_0 = \widehat{\mathbf{A}}\widehat{\mathbf{x}}_\star$. However, this contradicts case (i) of Lemma 1, which applies when deflated GMRES breaks down and says that $\widehat{\mathbf{x}}_\star \notin \widehat{\mathcal{K}}_n$.

Secondly, if $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant, we have in extension of (2.5) at the nth step

$$\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{P}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{V}_n = \mathbf{A}\mathbf{V}_n \,. \tag{3.2}$$

This implies that solving the system $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ with GMRES (and starting vector $\widehat{\mathbf{x}}_0 = \mathbf{o}$) is equivalent to solving $\mathbf{A}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ with GMRES. Since $\mathbf{A}$ is nonsingular, there are no breakdowns (described by Case (i) of Lemma 1), and ultimately the solution will be found (*i.e.*, Case (ii) will occur).

Finally, since $\mathcal{R}(\mathbf{V}_n) \subseteq \mathcal{Z}^\perp$ and the latter set is assumed to be $\mathbf{A}$–invariant, we have $\mathcal{R}(\mathbf{A}\mathbf{V}_n) \subseteq \mathbf{A}\mathcal{Z}^\perp = \mathcal{Z}^\perp$, so that $\mathbf{C}_n = \mathbf{Z}^{\mathsf{H}}\mathbf{A}\mathbf{V}_n = \mathbf{O}$. ☐

Eqs. (3.1) and (3.2) suggest that in the case where $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant we might apply GMRES with $\mathbf{A}$ instead of $\mathbf{P}\mathbf{A}$. But in some cases this might be risky due to round-off effects: round-off components in $\mathcal{Z}$ may grow fast since $\mathbf{A}^{-1}$ has large eigenvalues there.

Note that for $n = 0$ the breakdown condition $\widehat{\mathbf{r}}_0 \in \mathcal{N}(\widehat{\mathbf{A}})$ can be written as $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_0 \neq \{\mathbf{o}\}$, in accordance with the breakdown condition for the nth step.

The following simple 2×2 example taken from [31] exemplifies a breakdown in the first step:

$$\mathbf{A} :\equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{P} :\equiv \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{P}\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{r}_0 :\equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{3.3}$$

where $\widehat{\mathbf{A}} = \mathbf{PAP} = \mathbf{O}$ and $\mathbf{v}_0 = \widehat{\mathbf{r}}_0 = \mathbf{r}_0$, hence $\widehat{\mathbf{A}}\mathbf{v}_0 = \mathbf{o}$. So, $\mathcal{Z} = \mathcal{N}(\mathbf{P}) = \mathsf{span}\,\{\mathbf{e}_2\}$, $\mathcal{Z}^\perp = \mathsf{span}\,\{\mathbf{e}_1\}$, $\mathbf{v}_0 \in \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp$ here, and we have a breakdown in the first step.

We will generalize this example in the Appendix, where we will show that breakdowns are also possible at any later step up to $n = N - 1$.

Based on Theorem 2 we may formulate conditions that characterize the *possibility* of breakdowns in case of an unlucky choice of $\mathbf{x}_0$, that is, an unlucky $\widehat{\mathbf{r}}_0 \in \mathcal{Z}^\perp$.

COROLLARY 3. *Deflated* GMRES *can break down in the first Arnoldi step* (*for determining* $\mathbf{v}_1$) *if and only if the following four equivalent conditions hold:*

(1) $\mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp \neq \{\mathbf{o}\}$,
(2) $\mathbf{A}\mathcal{Z}^\perp \cap \mathcal{Z} \neq \{\mathbf{o}\}$,
(3) $\mathbf{A}\mathcal{Z}^\perp + \mathcal{Z} \neq \mathbb{C}^N$,
(4) $\mathsf{rank}\,\widehat{\mathbf{A}} < n - k$.

If these conditions are fulfilled for some given $\mathbf{A}$ *and* $\mathcal{Z}$, *then we can choose* $\mathbf{x}_0$ (*if* $\mathbf{b}$ *is given*), *so that* GMRES *breaks down in the first step.*

The equivalent Conditions (1)–(4) *are also necessary for deflated* GMRES *to break down in a later step.*

Conversely, a breakdown cannot occur in any step if equality holds in Conditions (1)–(4), *or, equivalently, if* $\mathcal{N}(\widehat{\mathbf{A}}) = \mathcal{Z}$, *that is, if* $\mathbf{A}\mathcal{Z}^\perp \oplus \mathcal{Z} = \mathbb{C}^N$.

Proof. According to Theorem 2, Condition (1) characterizes the possibility of a breakdown in the first step. It says that breakdowns are possible if and only if there exists $\mathbf{y} = \mathbf{P}\mathbf{y} \in \mathcal{Z}^\perp \backslash \{\mathbf{o}\}$ with $\mathbf{PAy} = \mathbf{PAPy} = \widehat{\mathbf{A}}\mathbf{y} = \mathbf{o}$, that is, with $\mathbf{o} \neq \mathbf{Ay} \in \mathcal{N}(\mathbf{P}) = \mathcal{Z}$. This is equivalent to Condition (2). Moreover, since $\mathsf{dim}\,\mathcal{Z} = k$ and $\mathsf{dim}\,\mathbf{A}\mathcal{Z}^\perp = \mathsf{dim}\,\mathcal{Z}^\perp = N - k$, the second condition is equivalent to the third one. Finally, $\mathcal{Z} = \mathcal{N}(\mathbf{P}) \subseteq \mathcal{N}(\widehat{\mathbf{A}})$ and therefore Condition (1) implies that $\mathsf{dim}\,\mathcal{N}(\widehat{\mathbf{A}}) > \mathsf{dim}\,\mathcal{Z} = k$, that is, $\mathsf{rank}\,\widehat{\mathbf{A}} < n - k$, and vice versa.

For a breakdown at step $n > 1$ we need, by Theorem 2, $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$. Since $\widehat{\mathcal{K}}_n \subseteq \mathsf{span}\,\{\widehat{\mathbf{r}}_0\} + \mathcal{R}(\widehat{\mathbf{A}}) \subseteq \mathcal{Z}^\perp$, Condition (1) must hold.

Conditions for the impossibility of breakdowns are obtained by negating the Conditions (1)–(4), noting that always $\mathcal{N}(\widehat{\mathbf{A}}) \supseteq \mathcal{Z}$, and observing the dimension statements given above. □

Finally, we point out the following fact.

COROLLARY 4. *The assumption that* $\mathcal{Z}^\perp$ *is* $\mathbf{A}$*-invariant is sufficient, but not necessary for guaranteeing that no breakdown can occur.*

Proof. Since $\mathbf{A}$ is nonsingular, $\mathcal{Z}^\perp$ is $\mathbf{A}$-invariant if and only if $\mathbf{A}\mathcal{Z}^\perp = \mathcal{Z}^\perp$. This condition means that on the left-hand side of the negated Condition (3) of Corollary 3 we have an orthogonal direct sum:

$$\mathbf{A}\mathcal{Z}^\perp \oplus \mathcal{Z} = \mathcal{Z}^\perp \oplus \mathcal{Z} = \mathbb{C}^N .$$

However, $\mathbf{A}\mathcal{Z}^\perp \oplus \mathcal{Z} = \mathbb{C}^N$ will hold whenever $\mathbf{A}\mathcal{Z}^\perp \cap \mathcal{Z} = \{\mathbf{o}\}$; hence, the condition that $\mathcal{Z}^\perp$ be $\mathbf{A}$-invariant appears not to be necessary for guaranteeing no breakdowns. The following example proves this claim. □

Example. We slightly modify the example of (3.3) by choosing

$$\mathbf{A} :\equiv \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{P} :\equiv \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{PA} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}, \quad \widehat{\mathbf{A}} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \mathbf{P} .$$

As before, $\mathcal{Z} = \mathsf{span}\,\{\mathbf{e}_2\}$, but now $\mathbf{A}\mathcal{Z}^\perp = \mathbf{A}\,\mathsf{span}\,\{\mathbf{e}_1\} = \mathsf{span}\,\{\mathbf{e}_1 + \mathbf{e}_2\} \neq \mathcal{Z}^\perp$. Hence, $\mathbf{A}\mathcal{Z}^\perp \oplus \mathcal{Z} = \mathbb{C}^2$. Consequently, for any $\widehat{\mathbf{r}}_0 = \mathbf{P}\mathbf{r}_0 \neq \mathbf{o}$ there will be no breakdown.

Remarks. (i) Note that when $\mathbf{A}$ is not Hermitian, then the property that $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant does not imply that $\mathcal{Z}$ is $\mathbf{A}$–invariant, and *vice versa*.

(ii) In case of a breakdown we might restart deflated GMRES with a new column $\mathbf{z}_{k+1} := \mathbf{v}_n$ appended to $\mathbf{Z}$. Repeating this measure if needed we will ultimately find a least square problem of type (2.11) with residual $\|\mathbf{r}_n\|_2 = 0$ and with, say, the original k replaced by $k+\ell$. However, we cannot find the approximate solution $\mathbf{x}_n$ from (2.7) unless we know the preimages $\mathbf{u}_{k+i}$ satisfying $\mathbf{v}_{k+i} = \mathbf{A}\mathbf{u}_{k+i}$, $i = 1, \ldots, \ell$.

(iii) Some further results on breakdowns of deflated GMRES and on how to avoid them in deflated MINRES are given in [31].[3]

4. Spectral deflation for symmetric problems. If $\mathbf{A}$ is Hermitian, then so is $\widehat{\mathbf{A}}$, and therefore the Arnoldi process can be replaced by a three-term symmetric Lanczos process, and the extended Hessenberg matrix $\underline{\mathbf{H}}_n$ of the previous section turns into an extended tridiagonal matrix $\underline{\mathbf{T}}_n$, for which a symmetric Lanczos relation

$$\mathbf{PAV}_n = \mathbf{V}_{n+1}\underline{\mathbf{T}}_n \tag{4.1}$$

holds and whose upper square part $\mathbf{T}_n$ is Hermitian. A *deflated* MINRES algorithm called *R*MINRES for the so simplified setting has been described in detail by Wang, de Sturler, and Paulino [62]. The same update procedure as in the original MINRES method [49] can be applied to find the QR decomposition of $\underline{\mathbf{T}}_n$. Wang *et al.* [62] also show that the approximate solutions $\mathbf{x}_n$ can still be updated by short recurrences. This is also seen from the fact stressed here and in [31] that the results of RMINRES can be found by solving first the projected problem $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$ in $\mathcal{Z}^\perp$ by MINRES and then adding to the solution a correction term in $\mathcal{Z}$; see Section 10.

In the Hermitian case the properties of deflated GMRES given in Theorem 2 and Corollary 3 persist and also hold for deflated MINRES. In particular, the possibility of a breakdown in the first step is still illustrated by the 2×2 example in (3.3). The possibility of a breakdown at a later step is still proven by the example in the Appendix, since the matrix $\mathbf{A}$ there is real symmetric.

We can reformulate the first part of Theorem 2 for deflated MINRES as follows.

THEOREM 5. *Let $\mathbf{A}$ be Hermitian; then so is $\widehat{\mathbf{A}}$. If $\widehat{\mathbf{r}}_0 \notin \mathcal{N}(\widehat{\mathbf{A}}) = \mathcal{R}(\widehat{\mathbf{A}})^\perp$, then as long as $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n = \{\mathbf{o}\}$, the deflated* MINRES *method obtained by adapting deflated* GMRES *to the symmetric case yields in the nth step the approximate solution $\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ whose residual $\mathbf{r}_n$ has minimal 2-norm.*

Conversely, if $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$ for some $n \geq 1$ then (and only then) deflated MINRES *breaks down in the nth step.*

Again, breakdowns cannot occur if $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant, and in this case the projected Lanczos relation (4.1) can be replaced by the Lanczos relation

$$\mathbf{AV}_n = \mathbf{V}_{n+1}\underline{\mathbf{T}}_n \,. \tag{4.2}$$

A special feature of the symmetric case is that $\mathcal{Z}^\perp$ is $\mathbf{A}$–invariant if and only if $\mathcal{Z}$ is $\mathbf{A}$–invariant. This is due to the fact that eigenspaces belonging to different eigenvalues are mutually orthogonal, and higher dimensional eigenspaces can be split up in mutually orthogonal ones if needed. The definition $\widehat{\mathbf{A}} = \mathbf{PAP}$ and the fact that $\mathbf{P}$ is the orthogonal projection onto $\mathcal{Z}^\perp$ yield then the following result on the spectral deflation of $\mathbf{A}$.

THEOREM 6. *Let $\mathbf{A}$ be Hermitian. If $\mathcal{Z}$ is $\mathbf{A}$–invariant, then $\mathcal{Z}^\perp$ is also $\mathbf{A}$–invariant and the restrictions of $\mathbf{A}$, $\widehat{\mathbf{A}}$, and $\mathbf{O}$ to $\mathcal{Z}$ and $\mathcal{Z}^\perp$ satisfy*

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}} = \mathbf{O}\big|_{\mathcal{Z}}\,, \qquad \widehat{\mathbf{A}}\big|_{\mathcal{Z}^\perp} = \mathbf{A}\big|_{\mathcal{Z}^\perp}\,. \tag{4.3}$$

[3] Note, however, that $\widehat{\mathbf{A}}$ is defined differently in [31].

Of course, (4.3) holds also if $\mathbf{A}$ is non-Hermitian, and, by chance, both $\mathcal{Z}$ and $\mathcal{Z}^\perp$ are $\mathbf{A}$-invariant.

5. Deflation by oblique projection: basic setting. So far we have based deflated GMRES and MINRES on orthogonal projections $\mathbf{Q}$ and $\mathbf{P} :\equiv \mathbf{I} - \mathbf{Q}$, but for GMRES and other solvers for nonsymmetric linear systems of equations it is more appropriate to consider oblique projections since the eigenspaces of $\mathbf{A}$ are typically not mutually orthogonal. Our approach is based on the natural splitting of $\mathbb{C}^N$ into the direct sum of two $\mathbf{A}$–invariant subspaces. In general, the corresponding decomposition of the residual search space will no longer be an orthogonal one. We therefore modify the setting of Section 2 as follows.

Let $\mathbf{U} \in \mathbb{C}^{N\times k}$ and $\widetilde{\mathbf{Z}} \in \mathbb{C}^{N\times k}$ have full rank k, and assume they are chosen such that the matrix $\mathbf{E}$ defined by

$$\mathbf{Z} :\equiv \mathbf{A}\mathbf{U}\,, \qquad \mathbf{E} :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{Z}$$

is nonsingular. Then set

$$\mathcal{U} :\equiv \mathcal{R}(\mathbf{U})\,, \qquad \mathcal{Z} :\equiv \mathcal{R}(\mathbf{Z}) = \mathbf{A}\mathcal{U}\,, \qquad \widetilde{\mathcal{Z}} :\equiv \mathcal{R}(\widetilde{\mathbf{Z}})\,,$$

and

$$\mathbf{Q} :\equiv \mathbf{Z}\mathbf{E}^{-1}\widetilde{\mathbf{Z}}^{\mathsf{H}}\,, \qquad \mathbf{P} :\equiv \mathbf{I} - \mathbf{Q} = \mathbf{I} - \mathbf{Z}\mathbf{E}^{-1}\widetilde{\mathbf{Z}}^{\mathsf{H}}\,. \tag{5.1}$$

Note that still $\mathbf{Q}^2 = \mathbf{Q}$ and $\mathbf{P}^2 = \mathbf{P}$, but now

$$\mathbf{Q}\mathcal{Z} = \mathcal{Z}\,, \qquad \mathbf{Q}\widetilde{\mathcal{Z}}^\perp = \{\mathbf{o}\}\,, \qquad \mathbf{P}\mathcal{Z} = \{\mathbf{o}\}\,, \qquad \mathbf{P}\widetilde{\mathcal{Z}}^\perp = \widetilde{\mathcal{Z}}^\perp\,, \tag{5.2}$$

where, as before, $\widetilde{\mathcal{Z}}^\perp$ denotes the orthogonal complement of $\widetilde{\mathcal{Z}}$. So, $\mathbf{Q}$ is the oblique projection onto $\mathcal{Z}$ along $\widetilde{\mathcal{Z}}^\perp$, while $\mathbf{P}$ is the oblique projection onto $\widetilde{\mathcal{Z}}^\perp$ along $\mathcal{Z}$. In particular, $\mathcal{N}(\mathbf{P}) = \mathcal{Z}$, $\mathcal{R}(\mathbf{P}) = \widetilde{\mathcal{Z}}^\perp$. Again, the subspaces $\mathcal{U}$ and $\mathcal{Z}$ will be used to augment the search spaces for the approximate solutions $\mathbf{x}_n$ and the corresponding residuals $\mathbf{r}_n$, respectively.

If the k columns $\widetilde{\mathbf{z}}_j$ of $\widetilde{\mathbf{Z}}$ are chosen biorthogonal to the k columns $\mathbf{z}_j$ of $\mathbf{Z}$, which means that these two sets of columns form dual bases of $\widetilde{\mathcal{Z}}$ and $\mathcal{Z}$, then $\mathbf{E} = \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{Z} = \mathbf{I}_k$ and the formulas for $\mathbf{Q}$ and $\mathbf{P}$ simplify as before:

$$\mathbf{Q} = \mathbf{Z}\widetilde{\mathbf{Z}}^{\mathsf{H}}\,, \qquad \mathbf{P} = \mathbf{I} - \mathbf{Q} = \mathbf{I} - \mathbf{Z}\widetilde{\mathbf{Z}}^{\mathsf{H}}\,. \tag{5.3}$$

Note that this is automatically true if we choose the columns of $\mathbf{Z}$ as (right-hand side) eigenvectors of $\mathbf{A}$ and the columns of $\widetilde{\mathbf{Z}}$ as the corresponding left eigenvectors. This property even generalizes to multiple eigenvalues and defective matrices if the eigenvectors are suitably chosen.

As in Section 2 we further let

$$\widehat{\mathbf{r}}_0 :\equiv \mathbf{P}\mathbf{r}_0\,, \qquad \widehat{\mathbf{A}} :\equiv \mathbf{P}\mathbf{A}\mathbf{P}\,.$$

Note that still

$$\mathcal{N}(\widehat{\mathbf{A}}) \supseteq \mathcal{N}(\mathbf{P}) = \mathcal{Z}\,, \qquad \mathcal{R}(\widehat{\mathbf{A}}) \subseteq \mathcal{R}(\mathbf{P}) = \widetilde{\mathcal{Z}}^\perp\,, \tag{5.4}$$

so that $\widehat{\mathbf{A}}|_{\widetilde{\mathcal{Z}}^\perp}$, the restriction of $\widehat{\mathbf{A}}$ to $\widetilde{\mathcal{Z}}^\perp$, is a possibly singular endomorphism of $\widetilde{\mathcal{Z}}^\perp$. Consequently, the Krylov subspaces $\widehat{\mathcal{K}}_n$ defined in (2.3) are all subsets of $\widetilde{\mathcal{Z}}^\perp$ since $\widehat{\mathbf{r}}_0 \in \widetilde{\mathcal{Z}}^\perp$. Therefore, we will be able to restrict a Krylov space solver to $\widetilde{\mathcal{Z}}^\perp$.

The reason for choosing this subspace lies in the following generalization of Theorem 6. Recall that a *simple* $\mathbf{A}$*–invariant subspace* is an $\mathbf{A}$–invariant subspace with the property that for any eigenvector it contains, it also contains all the other eigenvectors and generalized eigenvectors that belong to the same eigenvalue; see [58]. In other words, choosing a simple $\mathbf{A}$–invariant subspace induces a splitting of the characteristic polynomial into two co-prime factors and a related decomposition of the Jordan canonical form.

THEOREM 7. *Assume that $\mathcal{Z}$ is a simple k-dimensional $\mathbf{A}$–invariant subspace and $\widetilde{\mathcal{Z}}$ is the corresponding $\mathbf{A}^{\mathsf{H}}$–invariant subspace, that is, for any $\mathbf{Z}$, $\widetilde{\mathbf{Z}} \in \mathbb{C}^{N\times k}$ with $\mathcal{Z} = \mathcal{R}(\mathbf{Z})$ and $\widetilde{\mathcal{Z}} = \mathcal{R}(\widetilde{\mathbf{Z}})$ there are $\mathbf{G}$, $\widetilde{\mathbf{G}} \in \mathbb{C}^{k\times k}$ such that, with $\mathbf{E} :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{Z}$,*

$$\mathbf{A}\mathbf{Z} = \mathbf{Z}\mathbf{G}\,, \qquad \mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{Z}} = \widetilde{\mathbf{Z}}\widetilde{\mathbf{G}}\,, \qquad \widetilde{\mathbf{G}} = \mathbf{E}^{-\mathsf{H}}\mathbf{G}^{\mathsf{H}}\mathbf{E}^{\mathsf{H}}\,. \tag{5.5}$$

Then $\widetilde{\mathcal{Z}}^{\perp}$ is also $\mathbf{A}$–invariant and $\mathcal{Z} \oplus \widetilde{\mathcal{Z}}^{\perp} = \mathbb{C}^N$. Moreover, the restrictions of $\mathbf{A}$, $\widehat{\mathbf{A}}$, and $\mathbf{O}$ to $\mathcal{Z}$ and $\widetilde{\mathcal{Z}}^{\perp}$ satisfy

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}} = \mathbf{O}\big|_{\mathcal{Z}}\,, \qquad \widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}} = \mathbf{A}\big|_{\widetilde{\mathcal{Z}}^{\perp}}\,. \tag{5.6}$$

Proof. To fix our mind, let us first choose a special basis for $\mathcal{Z}$ and assume that $\mathbf{A}$ has a Jordan decomposition

$$\mathbf{A}\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_{\perp} \end{bmatrix} = \begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_{\perp} \end{bmatrix}\begin{bmatrix} \mathbf{J} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_{\perp} \end{bmatrix}, \tag{5.7}$$

where despite our notation $\widetilde{\mathbf{Z}}_{\perp}$ is at this point not yet known to be related to $\widetilde{\mathcal{Z}}^{\perp}$. Eqn. (5.7) just reflects the fact that $\mathcal{Z}$ is $\mathbf{A}$–invariant in the assumed sense, that $\mathbf{J}$ is the Jordan canonical form of $\mathbf{A}\big|_{\mathcal{Z}}$, and that $\mathbf{Z}$ contains the corresponding eigenvectors and generalized eigenvectors, while $\mathbf{J}_{\perp}$ is the Jordan canonical form of $\mathbf{A}\big|_{\mathcal{R}(\widetilde{\mathbf{Z}}_{\perp})}$ and the columns of $\widetilde{\mathbf{Z}}_{\perp}$ are the corresponding eigenvectors and generalized eigenvectors. So, $\widetilde{\mathbf{Z}}_{\perp}$ just consists of the 'remaining' eigenvectors and generalized eigenvectors and $\mathbf{J}_{\perp}$ consists of the 'remaining' Jordan blocks. Clearly, $\mathcal{R}(\widetilde{\mathbf{Z}}_{\perp})$ is also an $\mathbf{A}$–invariant subspace, and $\mathcal{Z} \oplus \mathcal{R}(\widetilde{\mathbf{Z}}_{\perp})$ is a direct sum, but in general not an orthogonal one. (Actually we could weaken the assumption: we need the separation of the Jordan blocks of $\mathbf{A}$ into two sets, but we need not that the eigenvalues are necessarily different in the two sets.)

As is well-known, the rows of the inverse of $\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_{\perp} \end{bmatrix}$ are the left-hand side eigenvectors and generalized eigenvectors of $\mathbf{A}$, or, equivalently, the complex conjugate of the right-hand side eigenvectors and generalized eigenvectors of $\mathbf{A}^{\mathsf{H}}$. To allow for another pair of bases for the induced pair of invariant subspaces of $\mathbf{A}^{\mathsf{H}}$, we let, for some nonsingular $\mathbf{E}$ and $\mathbf{E}_{\perp} \in \mathbb{C}^{k\times k}$,

$$\begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}} \\ \mathbf{Z}_{\perp}^{\mathsf{H}} \end{bmatrix} :\equiv \begin{bmatrix} \mathbf{E} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_{\perp} \end{bmatrix}\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_{\perp} \end{bmatrix}^{-1}, \tag{5.8}$$

so that $\mathbf{E} :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{Z}$ as before, and, in addition,

$$\mathbf{E}_{\perp} :\equiv \mathbf{Z}_{\perp}^{\mathsf{H}}\widetilde{\mathbf{Z}}_{\perp}\,, \qquad \widetilde{\mathbf{Z}}^{\mathsf{H}}\widetilde{\mathbf{Z}}_{\perp} = \mathbf{O}_{k\times(N-k)}\,, \qquad \mathbf{Z}_{\perp}^{\mathsf{H}}\mathbf{Z} = \mathbf{O}_{(N-k)\times k}\,.$$

From the last two equations it follows that indeed $\mathcal{R}(\mathbf{Z}_{\perp}) = \mathcal{Z}^{\perp}$ and $\mathcal{R}(\widetilde{\mathbf{Z}}_{\perp}) = \widetilde{\mathcal{Z}}^{\perp}$, and by (5.7) the latter space was seen to be $\mathbf{A}$–invariant. Moreover, multiplying (5.7) from both sides with the inverse of $\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_{\perp} \end{bmatrix}$ and inserting (5.8) yields

$$\begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}} \\ \mathbf{Z}_{\perp}^{\mathsf{H}} \end{bmatrix}\mathbf{A} = \begin{bmatrix} \mathbf{E} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_{\perp} \end{bmatrix}\begin{bmatrix} \mathbf{J} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_{\perp} \end{bmatrix}\begin{bmatrix} \mathbf{E}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_{\perp}^{-1} \end{bmatrix}\begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}} \\ \mathbf{Z}_{\perp}^{\mathsf{H}} \end{bmatrix}. \tag{5.9}$$

So, the complex-conjugate of the columns of $\widetilde{\mathcal{Z}}$ and $\mathcal{Z}^\perp$ span left-invariant subspaces. Finally, taking the Hermitian transpose leads to

$$\mathbf{A}^\mathsf{H} \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} \begin{bmatrix} \mathbf{E}^{-\mathsf{H}} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_\perp^{-\mathsf{H}} \end{bmatrix} \begin{bmatrix} \mathbf{J}^\mathsf{H} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_\perp^\mathsf{H} \end{bmatrix} \begin{bmatrix} \mathbf{E}^\mathsf{H} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_\perp^\mathsf{H} \end{bmatrix}, \tag{5.10}$$

which implies in particular that $\mathbf{A}^\mathsf{H}\widetilde{\mathbf{Z}} = \widetilde{\mathbf{Z}}\mathbf{E}^{-\mathsf{H}}\mathbf{J}^\mathsf{H}\mathbf{E}^\mathsf{H}$. This establishes (5.5) in the case where $\mathbf{G} = \mathbf{J}$ and $\widetilde{\mathbf{G}} = \mathbf{E}^{-\mathsf{H}}\mathbf{J}^\mathsf{H}\mathbf{E}^\mathsf{H}$. The general case of $\mathbf{G}$ and $\widetilde{\mathbf{G}}$ follows by noting that we did nowhere make any use of the Jordan structure of $\mathbf{J}$ and $\mathbf{J}_\perp$, but only of the 2×2 block diagonal structure in (5.7), that is, we referred to the Jordan structure just to ease the discussion.

On the other hand, when indeed starting from a Jordan decomposition (5.7) of $\mathbf{A}$ and choosing $\widetilde{\mathbf{Z}}$ and $\mathbf{Z}_\perp$ so that $\mathbf{E} = \mathbf{I}_k$ and $\mathbf{E}_\perp = \mathbf{I}_{N-k}$, we turn (5.10) into a Jordan decomposition (with lower bidiagonal Jordan blocks) of $\mathbf{A}^\mathsf{H}$.

Finally, it follows from (5.7) and the properties of $\mathbf{P}$ that

$$\begin{aligned} \widehat{\mathbf{A}} \begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix} &= \mathbf{PAP} \begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix} = \mathbf{PA} \begin{bmatrix} \mathbf{O} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix} \\ &= \mathbf{P} \begin{bmatrix} \mathbf{O} & \widetilde{\mathbf{Z}}_\perp \mathbf{J}_\perp \end{bmatrix} = \begin{bmatrix} \mathbf{O} & \widetilde{\mathbf{Z}}_\perp \mathbf{J}_\perp \end{bmatrix}. \end{aligned} \tag{5.11}$$

So, $\widehat{\mathbf{A}}\mathbf{Z} = \mathbf{O}$, and by comparison with (5.7) we find $\widehat{\mathbf{A}}\widetilde{\mathbf{Z}}_\perp = \widetilde{\mathbf{Z}}_\perp\mathbf{J}_\perp = \mathbf{A}\widetilde{\mathbf{Z}}_\perp$, which proves (5.6). □

But also in the typical situation where $\mathcal{Z}$ and $\widetilde{\mathcal{Z}}^\perp$ are not $\mathbf{A}$–invariant this pair of spaces is well chosen, as the following simple fact underlines.

LEMMA 8. *Let* $\mathbf{Z}$, $\widetilde{\mathbf{Z}} \in \mathbb{C}^{N\times k}$ *be given such that* $\mathbf{E} :\equiv \widetilde{\mathbf{Z}}^\mathsf{H}\mathbf{Z}$ *is nonsingular, let* $\mathcal{Z} :\equiv \mathcal{R}(\mathbf{Z})$ *and* $\widetilde{\mathcal{Z}} :\equiv \mathcal{R}(\widetilde{\mathbf{Z}})$*, and choose* $\mathbf{Z}_\perp$, $\widetilde{\mathbf{Z}}_\perp \in \mathbb{C}^{N\times(N-k)}$ *such that their columns consist of bases of the orthogonal complements* $\mathcal{Z}^\perp$ *and* $\widetilde{\mathcal{Z}}^\perp$*, respectively. Then*

$$\begin{bmatrix} \widetilde{\mathbf{Z}}^\mathsf{H} \\ \mathbf{Z}_\perp^\mathsf{H} \end{bmatrix} \begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix} = \begin{bmatrix} \mathbf{E} & \mathbf{O} \\ \mathbf{O} & \mathbf{E}_\perp \end{bmatrix}, \tag{5.12}$$

where all three matrices are nonsingular. In particular, $\mathbf{E}_\perp$ *is nonsingular too, and*

$$\mathcal{Z} \oplus \widetilde{\mathcal{Z}}^\perp = \widetilde{\mathcal{Z}} \oplus \mathcal{Z}^\perp = \mathbb{C}^N \tag{5.13}$$

are both decompositions of $\mathbb{C}^N$ *into (in general nonorthogonal) complements.*

Proof. The block diagonal structure of the right-hand side of (5.12) holds by definition of $\mathbf{Z}_\perp$ and $\widetilde{\mathbf{Z}}_\perp$, but we need to show that on the left-hand side the matrices $\begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix}$ and $\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix}$ are nonsingular, *i.e.*, their columns are linearly independent.

Let $\mathbf{z}_\perp$ be any nonzero element of $\mathcal{Z}^\perp$. So, $\mathbf{Z}^\mathsf{H}\mathbf{z}_\perp = \mathbf{o}$ and $\mathbf{z}_\perp \neq \mathbf{o}$. For a proof by contradiction, let us assume that $\mathbf{z}_\perp$ is a linear combination of columns of $\widetilde{\mathbf{Z}}$, *i.e.*, $\mathbf{z}_\perp = \widetilde{\mathbf{Z}}\mathbf{k}$ for some $\mathbf{k} \in \mathbb{C}^{N-k}$. Then,

$$\mathbf{o} = \mathbf{Z}^\mathsf{H}\mathbf{z}_\perp = \mathbf{Z}^\mathsf{H}\widetilde{\mathbf{Z}}\mathbf{k} = \mathbf{E}^\mathsf{H}\mathbf{k},$$

which implies that $\mathbf{k} = \mathbf{o}$, and thus $\mathbf{z}_\perp = \mathbf{o}$ in contrast to our assumption. It follows that $\widetilde{\mathcal{Z}} \cap \mathcal{Z}^\perp = \{\mathbf{o}\}$. An analogue argument shows that $\mathcal{Z} \cap \widetilde{\mathcal{Z}}^\perp = \{\mathbf{o}\}$. □

Remark. Note that, by definition, $\mathcal{Z} \oplus \mathcal{Z}^\perp = \widetilde{\mathcal{Z}} \oplus \widetilde{\mathcal{Z}}^\perp = \mathbb{C}^N$ are two other decompositions of $\mathbb{C}^N$, and they even feature orthogonal complements. In contrast, in general, the decompositions in (5.13) are not orthogonal, but they are adapted to the operator $\mathbf{A}$ if $\mathbf{Z}$ is exactly or nearly $\mathbf{A}$–invariant. In (5.7) we assumed that $\mathbf{Z}$ and $\widetilde{\mathbf{Z}}_\perp$ contain eigenvectors and generalized eigenvectors, which, in general, is not true in the setting of this and the following sections. In general, we will have

$$\mathbf{A}\begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix} = \begin{bmatrix} \mathbf{Z} & \widetilde{\mathbf{Z}}_\perp \end{bmatrix}\begin{bmatrix} \mathbf{G}_{11} & \mathbf{G}_{12} \\ \mathbf{G}_{21} & \mathbf{G}_{22} \end{bmatrix}, \tag{5.14}$$

where the blocks $\mathbf{G}_{12}$ and $\mathbf{G}_{21}$ can be expected to contain only small elements if $\mathcal{Z}$ and $\widetilde{\mathcal{Z}}^\perp$ are nearly $\mathbf{A}$–invariant.

6. Deflation by oblique projection: truly deflated GMRES. Let us now come to the details of a correctly deflated GMRES based on the observations of the previous section. Given an initial guess $\mathbf{x}_0$, we choose as in Section 2 iterates $\mathbf{x}_n$ from

$$\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}\,, \tag{6.1}$$

where the Krylov subspaces $\widehat{\mathcal{K}}_n$ are still defined by (2.3). This implies that

$$\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{A}\mathbf{x}_0 \in \mathbf{r}_0 + \mathbf{A}\widehat{\mathcal{K}}_n + \mathcal{Z}\,. \tag{6.2}$$

We again construct a nested sequence of orthogonal bases for the Krylov subspaces $\widehat{\mathcal{K}}_n$ by an Arnoldi process started with $\mathbf{v}_0 :\equiv \widehat{\mathbf{r}}_0/\beta$, where now $\widehat{\mathbf{r}}_0 :\equiv \mathbf{P}\mathbf{r}_0 \in \widetilde{\mathcal{Z}}^\perp$ and $\beta :\equiv \|\widehat{\mathbf{r}}_0\|_2$. As before, this is expressed by the Arnoldi relation $\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n$. Since $\mathcal{R}(\mathbf{V}_n) = \widehat{\mathcal{K}}_n \subseteq \widetilde{\mathcal{Z}}^\perp$, we have $\mathbf{P}\mathbf{V}_n = \mathbf{V}_n$, and therefore again

$$\widehat{\mathbf{A}}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{P}\mathbf{V}_n = \mathbf{P}\mathbf{A}\mathbf{V}_n\,, \tag{6.3}$$

so that the Arnoldi relation still simplifies to

$$\mathbf{P}\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n\,. \tag{6.4}$$

However, recall that $\mathbf{P}$ and, hence, $\widehat{\mathbf{A}}$ are now defined differently.

In view of (6.1) we represent $\mathbf{x}_n$ again as

$$\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n + \mathbf{U}\mathbf{m}_n \tag{6.5}$$

with coordinate vectors $\mathbf{k}_n \in \mathbb{C}^n$ and $\mathbf{m}_n \in \mathbb{C}^k$. Regarding the residuals, where we prefer a representation in terms of an orthonormal basis, we note that $\mathbf{Z}$ cannot be expected to have such columns, whence we propose to QR-decompose $\mathbf{Z}$ first:

$$\mathbf{Z} = \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\,, \qquad \mathbf{Z}_\circ^{\mathsf{H}}\mathbf{Z}_\circ = \mathbf{I}_k\,. \tag{6.6}$$

Then, after inserting $\mathbf{A}\mathbf{U} = \mathbf{Z} = \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}$, we get

$$\mathbf{r}_n = \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\mathbf{m}_n\,. \tag{6.7}$$

Due to the Arnoldi relation (6.4) and the decomposition $\mathbf{r}_0 = \widehat{\mathbf{r}}_0 + \mathbf{Q}\mathbf{r}_0 = \mathbf{v}_0\beta + \mathbf{Q}\mathbf{r}_0$ this becomes now, with $\mathbf{Q} = \mathbf{Z}\widetilde{\mathbf{Z}}^{\mathsf{H}} = \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\widetilde{\mathbf{Z}}^{\mathsf{H}}$ and $\mathbf{C}_n :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{A}\mathbf{V}_n$,

$$\begin{aligned}
\mathbf{r}_n &= \mathbf{v}_0\beta + \mathbf{Q}\mathbf{r}_0 - (\mathbf{P}+\mathbf{Q})\mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\mathbf{m}_n \\
&= \mathbf{v}_0\beta + \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{V}_{n+1}\underline{\mathbf{H}}_n\mathbf{k}_n - \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}\mathbf{m}_n \\
&= \begin{bmatrix} \mathbf{Z}_\circ & \mathbf{V}_{n+1} \end{bmatrix}\underline{\mathbf{q}}_n\,,
\end{aligned} \tag{6.8}$$

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where

$$\underline{\mathbf{q}}_n :\equiv \begin{bmatrix} \mathbf{q}_n^{\circ} \\ \underline{\mathbf{q}}_n^{\perp} \end{bmatrix} :\equiv \begin{bmatrix} \mathbf{R}_{\mathsf{QR}}\widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 \\ \underline{\mathbf{e}}_1\beta \end{bmatrix} - \begin{bmatrix} \mathbf{R}_{\mathsf{QR}} & \mathbf{R}_{\mathsf{QR}}\mathbf{C}_n \\ \mathbf{O} & \underline{\mathbf{H}}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} \in \mathbb{C}^{k+n+1} \tag{6.9}$$

is the *truly deflated* GMRES *quasi-residual*.

The columns of each $\mathbf{Z}_{\circ}$ and $\mathbf{V}_{n+1}$ are still orthonormal, but those of $\mathbf{Z}_{\circ}$ need no longer be orthogonal to those of $\mathbf{V}_{n+1}$. So, in general, $\|\mathbf{r}_n\|_2 \neq \|\underline{\mathbf{q}}_n\|_2$, but since

$$\mathbf{r}_n = \mathbf{Z}_{\circ}\mathbf{q}_n^{\circ} + \mathbf{V}_{n+1}\underline{\mathbf{q}}_n^{\perp} \qquad \text{with} \quad \mathbf{Z}_{\circ}\mathbf{q}_n^{\circ} = \mathbf{Q}\mathbf{r}_n \in \mathcal{Z}\,, \quad \mathbf{V}_{n+1}\underline{\mathbf{q}}_n^{\perp} = \mathbf{P}\mathbf{r}_n \in \widetilde{\mathcal{Z}}^{\perp} \tag{6.10}$$

we have at least

$$\|\underline{\mathbf{q}}_n\|_2^2 = \|\mathbf{q}_n^{\circ}\|_2^2 + \|\underline{\mathbf{q}}_n^{\perp}\|_2^2 = \|\mathbf{Q}\mathbf{r}_n\|_2^2 + \|\mathbf{P}\mathbf{r}_n\|_2^2\,. \tag{6.11}$$

It is therefore tempting to minimize $\|\underline{\mathbf{q}}_n\|_2$ instead of $\|\mathbf{r}_n\|_2$, and as in Section 2 this amounts to solving an $n \times (n+1)$ least squares problem with the extended Hessenberg matrix $\underline{\mathbf{H}}_n$ for minimizing $\|\mathbf{q}_n^{\perp}\|_2$, that is, for finding $\mathbf{k}_n$ and subsequently choosing $\mathbf{m}_n$ such that $\mathbf{q}_n^{\circ} = \mathbf{o}$:

$$\min \|\underline{\mathbf{q}}_n\|_2 = \min \|\underline{\mathbf{q}}_n^{\perp}\|_2 = \min_{\mathbf{k}_n \in \mathbb{C}^n} \|\underline{\mathbf{e}}_1\beta - \underline{\mathbf{H}}_n\mathbf{k}_n\|_2\,, \qquad \mathbf{m}_n := \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n\,. \tag{6.12}$$

At this point we see that the QR decomposition of $\mathbf{Z}$ is actually not needed since we can achieve that $\mathbf{q}_n^{\circ} = \mathbf{o}$ and thus $\mathbf{Z}_{\circ}\mathbf{q}_n^{\circ} = \mathbf{o}$. In other words, we can represent $\mathbf{r}_n$ as

$$\mathbf{r}_n = \begin{bmatrix} \mathbf{Z} & \mathbf{V}_{n+1} \end{bmatrix} \widehat{\underline{\mathbf{q}}}_n \tag{6.13}$$

with

$$\widehat{\underline{\mathbf{q}}}_n :\equiv \begin{bmatrix} \mathbf{q}_n^{\mathsf{Z}} \\ \underline{\mathbf{q}}_n^{\perp} \end{bmatrix} :\equiv \begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 \\ \underline{\mathbf{e}}_1\beta \end{bmatrix} - \begin{bmatrix} \mathbf{I} & \mathbf{C}_n \\ \mathbf{O} & \underline{\mathbf{H}}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} \in \mathbb{C}^{k+n+1} \tag{6.14}$$

and are then lead to the same solution as given by (6.12). Formally there is very little difference between this algorithm and the one of Section 2, but there is an essential mathematical improvement regarding the deflation of $\mathbf{A}$. In view of Theorem 7 we call the new algorithm *truly deflated* GMRES.

In practice, this algorithm will be applied with restarts, and the matrices $\mathbf{Z}$ and $\widetilde{\mathbf{Z}}$ with the approximate right and left eigenvectors may be updated at each restart.

Truly deflated GMRES can break down in the same way as deflated GMRES. Here is the adaptation of Theorem 2, which only requires very small changes.

THEOREM 9. *If $\widehat{\mathbf{r}}_0 \notin \mathcal{N}(\widehat{\mathbf{A}})$, then as long as $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n = \{\mathbf{o}\}$, the truly deflated* GMRES *method defined by* (6.4)–(6.5), (6.9), *and* (6.12) *yields in the nth step the approximate solution $\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ whose quasi-residual $\underline{\mathbf{q}}_n$ defined by* (6.9) *has minimal* 2*-norm.*

However, if $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widetilde{\mathcal{Z}}^{\perp} \neq \{\mathbf{o}\}$ and if $\mathbf{x}_0$ is chosen such that $\widehat{\mathbf{r}}_0 \in \mathcal{N}(\widehat{\mathbf{A}})$, then (and only then) truly deflated GMRES *breaks down in the first step where $n = 1$. Moreover, at step $n > 1$, if (and only if) $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$, the method breaks down when attempting to construct $\mathbf{v}_n$. In case of a breakdown, the search space $\mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ does not contain the exact solution $\mathbf{x}_\star$.*

If $\widetilde{\mathcal{Z}}^{\perp}$ is $\mathbf{A}$–invariant, breakdowns cannot happen, $\mathbf{C}_n = \mathbf{O}$, and the Arnoldi relation (6.4) *can be replaced by*

$$\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n\,. \tag{6.15}$$

Proof. Essentially we just have to replace in the proof of Theorem 2 every occurrence of $\mathcal{Z}^{\perp}$ by $\widetilde{\mathcal{Z}}^{\perp}$. This applies also to the last sentence, including (6.15). In that proof we only made use of $\mathcal{Z}$ and $\mathcal{Z}^{\perp}$ being complimentary subspaces, but not of their orthogonality. ☐

Corollaries 3 and 4 can also be adapted easily.

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7. Deflation by oblique projection: the adjoint Krylov space. Some very efficient, computing time and memory space reducing alternatives to GMRES are based on the nonsymmetric Lanczos biorthogonalization process. Our aim of the next two sections is to adapt the approach of the previous two sections to these alternatives, in particular to the quasi-minimal residual (QMR) method of Freund and Nachtigal [28], which is fully analogous to GMRES. To this end, we first need to look at the adjoints of the projections $\mathbf{Q}$ and $\mathbf{P}$ of (5.1) and the adjoint of our restricted operator $\widehat{\mathbf{A}} :\equiv \mathbf{PAP}$.

The adjoint projections are defined by

$$\mathbf{Q}^{\mathsf{H}} :\equiv \widetilde{\mathbf{Z}}\mathbf{E}^{-\mathsf{H}}\mathbf{Z}^{\mathsf{H}}, \qquad \mathbf{P}^{\mathsf{H}} :\equiv \mathbf{I} - \mathbf{Q}^{\mathsf{H}} = \mathbf{I} - \widetilde{\mathbf{Z}}\mathbf{E}^{-\mathsf{H}}\mathbf{Z}^{\mathsf{H}}, \tag{7.1}$$

from which we see that the properties (5.2) of $\mathbf{Q}$ and $\mathbf{P}$ are supplemented as follows:

$$\mathbf{Q}\mathcal{Z} = \mathcal{Z}, \qquad \mathbf{Q}\widetilde{\mathcal{Z}}^{\perp} = \{\mathbf{o}\}, \qquad \mathbf{P}\mathcal{Z} = \{\mathbf{o}\}, \qquad \mathbf{P}\widetilde{\mathcal{Z}}^{\perp} = \widetilde{\mathcal{Z}}^{\perp}, \tag{7.2a}$$

$$\mathbf{Q}^{\mathsf{H}}\widetilde{\mathcal{Z}} = \widetilde{\mathcal{Z}}, \qquad \mathbf{Q}^{\mathsf{H}}\mathcal{Z}^{\perp} = \{\mathbf{o}\}, \qquad \mathbf{P}^{\mathsf{H}}\widetilde{\mathcal{Z}} = \{\mathbf{o}\}, \qquad \mathbf{P}^{\mathsf{H}}\mathcal{Z}^{\perp} = \mathcal{Z}^{\perp}. \tag{7.2b}$$

So, $\mathbf{Q}^{\mathsf{H}}$ is the oblique projection onto $\widetilde{\mathcal{Z}}$ along $\mathcal{Z}^{\perp}$, while $\mathbf{P}^{\mathsf{H}}$ is the oblique projection onto $\mathcal{Z}^{\perp}$ along $\widetilde{\mathcal{Z}}$. In particular,

$$\mathcal{N}(\mathbf{P}) = \mathcal{Z}, \qquad \mathcal{N}(\mathbf{P}^{\mathsf{H}}) = \widetilde{\mathcal{Z}}, \qquad \mathcal{R}(\mathbf{P}) = \widetilde{\mathcal{Z}}^{\perp}, \qquad \mathcal{R}(\mathbf{P}^{\mathsf{H}}) = \mathcal{Z}^{\perp}. \tag{7.3}$$

For the adjoint operator $\widehat{\mathbf{A}}^{\mathsf{H}} = \mathbf{P}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}^{\mathsf{H}}$ this means that

$$\mathcal{N}(\widehat{\mathbf{A}}^{\mathsf{H}}) \supseteq \mathcal{N}(\mathbf{P}^{\mathsf{H}}) = \widetilde{\mathcal{Z}}, \qquad \mathcal{R}(\widehat{\mathbf{A}}^{\mathsf{H}}) \subseteq \mathcal{R}(\mathbf{P}^{\mathsf{H}}) = \mathcal{Z}^{\perp}, \tag{7.4}$$

We define the dual Krylov subspaces (sometimes called the shadow spaces) started from $\widetilde{\mathbf{v}}_0 \in \mathcal{Z}^{\perp}$ by

$$\widehat{\mathcal{L}}_n :\equiv \mathcal{K}_n(\widehat{\mathbf{A}}^{\mathsf{H}}, \widetilde{\mathbf{v}}_0) :\equiv \mathsf{span}\,\{\widetilde{\mathbf{v}}_0, \widehat{\mathbf{A}}^{\mathsf{H}}\widetilde{\mathbf{v}}_0, \ldots, (\widehat{\mathbf{A}}^{\mathsf{H}})^{n-1}\widetilde{\mathbf{v}}_0\} \subseteq \mathcal{Z}^{\perp}. \tag{7.5}$$

Methods based on implicitly or explicitly constructing for each n a pair of biorthogonal bases should choose the right and left bases, respectively, such that

$$\mathcal{R}\left(\begin{bmatrix} \mathbf{Z} & \mathbf{V}_n \end{bmatrix}\right) = \mathcal{Z} \oplus \widehat{\mathcal{K}}_{n+1} \subseteq \mathcal{Z} \oplus \widetilde{\mathcal{Z}}^{\perp} = \mathbb{C}^N, \tag{7.6a}$$

$$\mathcal{R}\left(\begin{bmatrix} \widetilde{\mathbf{Z}} & \widetilde{\mathbf{V}}_n \end{bmatrix}\right) = \widetilde{\mathcal{Z}} \oplus \widehat{\mathcal{L}}_{n+1} \subseteq \widetilde{\mathcal{Z}} \oplus \mathcal{Z}^{\perp} = \mathbb{C}^N. \tag{7.6b}$$

In the rest of this section let us again consider the case where $\mathbf{Z}$ is $\mathbf{A}$–invariant, which led to Theorem 7 and motivated using deflated solvers in the first place. Theorem 7 translates to the adjoint operator as follows.

THEOREM 10. *Under the assumptions of Theorem 7, $\widetilde{\mathcal{Z}}$ and $\mathcal{Z}^{\perp}$ are $\mathbf{A}^{\mathsf{H}}$–invariant, and the restrictions of $\mathbf{A}^{\mathsf{H}}$, $\widehat{\mathbf{A}}^{\mathsf{H}}$, and $\mathbf{O}$ to $\widetilde{\mathcal{Z}}$ and $\mathcal{Z}^{\perp}$ satisfy*

$$\widehat{\mathbf{A}}^{\mathsf{H}}\big|_{\widetilde{\mathcal{Z}}} = \mathbf{O}\big|_{\widetilde{\mathcal{Z}}}, \qquad \widehat{\mathbf{A}}^{\mathsf{H}}\big|_{\mathcal{Z}^{\perp}} = \mathbf{A}^{\mathsf{H}}\big|_{\mathcal{Z}^{\perp}}. \tag{7.7}$$

Proof. We take $\mathbf{Z}$ and $\widetilde{\mathbf{Z}}_{\perp}$ as given by the Jordan decomposition (5.7), and choose $\widetilde{\mathbf{Z}}$ and $\mathbf{Z}_{\perp}$, as towards the end of the proof of Theorem 7, such that $\mathbf{E} = \mathbf{I}_k$ and $\mathbf{E}_{\perp} = \mathbf{I}_{N-k}$. Then, (5.9) simplifies to

$$\begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}} \\ \mathbf{Z}_{\perp}^{\mathsf{H}} \end{bmatrix} \mathbf{A} = \begin{bmatrix} \mathbf{J} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_{\perp} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{Z}}^{\mathsf{H}} \\ \mathbf{Z}_{\perp}^{\mathsf{H}} \end{bmatrix}, \tag{7.8}$$

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while (5.10) becomes

$$\mathbf{A}^{\mathsf{H}} \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} \begin{bmatrix} \mathbf{J}^{\mathsf{H}} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_\perp^{\mathsf{H}} \end{bmatrix} . \tag{7.9}$$

From the proof of Theorem 7 we know already that $\widetilde{\mathbf{Z}}$ and $\mathbf{Z}_\perp$ contain in their columns bases of $\widetilde{\mathcal{Z}}$ and $\mathcal{Z}^\perp$, respectively; so these two spaces are $\mathbf{A}^{\mathsf{H}}$–invariant. Finally, in analogy to (5.11) we have

$$\begin{aligned} \widehat{\mathbf{A}}^{\mathsf{H}} \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} &= \mathbf{P}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\mathbf{P}^{\mathsf{H}} \begin{bmatrix} \widetilde{\mathbf{Z}} & \mathbf{Z}_\perp \end{bmatrix} = \mathbf{P}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}} \begin{bmatrix} \mathbf{O} & \mathbf{Z}_\perp \end{bmatrix} \\ &= \mathbf{P}^{\mathsf{H}} \begin{bmatrix} \mathbf{O} & \mathbf{Z}_\perp \mathbf{J}_\perp^{\mathsf{H}} \end{bmatrix} = \begin{bmatrix} \mathbf{O} & \mathbf{Z}_\perp \mathbf{J}_\perp^{\mathsf{H}} \end{bmatrix} , \end{aligned} \tag{7.10}$$

from which, by comparison with (7.9), we find the result (7.7). □

8. Deflation by oblique projection: deflated QMR. Now we are ready to introduce a *deflated QMR* method that is analogous to our truly deflated GMRES, but replaces the Arnoldi process by the nonsymmetric Lanczos process. The latter has the important feature that it can provide approximations of both right and left eigenvectors. For details about the QMR method, see Freund and Nachtigal [28]; for a presentation in the notation used here[4], see [32]. Deflated QMR is started with the pair

$$\mathbf{v}_0 :\equiv \widehat{\mathbf{r}}_0/\beta = \mathbf{P}\mathbf{r}_0/\beta\,, \quad \beta :\equiv \|\widehat{\mathbf{r}}_0\|\,, \tag{8.1}$$

$$\widetilde{\mathbf{v}}_0 :\equiv \widetilde{\mathbf{r}}_0/\widetilde{\beta}\,, \qquad \widetilde{\beta} :\equiv \|\widetilde{\mathbf{r}}_0\|\,, \tag{8.2}$$

where $\widetilde{\mathbf{r}}_0$ must be chosen such that $\widetilde{\mathbf{r}}_0 \in \mathcal{Z}^\perp$ and $\widetilde{\mathbf{r}}_0^{\mathsf{H}}\widehat{\mathbf{r}}_0 \neq 0$. The Arnoldi relation (6.4) is then replaced by a pair of Lanczos relations

$$\mathbf{P}\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{T}}_n\,, \qquad \mathbf{P}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{V}}_n = \widetilde{\mathbf{V}}_{n+1}\underline{\widetilde{\mathbf{T}}}_n\,, \tag{8.3}$$

where we may enforce that all columns of $\mathbf{V}_{n+1}$ and $\widetilde{\mathbf{V}}_{n+1}$ have 2-norm one, and where

$$\mathbf{D}_{n+1} :\equiv \widetilde{\mathbf{V}}_{n+1}^{\mathsf{H}}\mathbf{V}_{n+1}$$

is nonsingular diagonal or, if look-ahead steps [26] are needed, block-diagonal. With this choice (7.6a) and (7.6b) hold.

So, if we start again from the ansatz (6.5) for the approximate solutions $\mathbf{x}_n$, which implies the representation (6.7) for the residuals, and if we again QR-decompose $\mathbf{A}\mathbf{U} = \mathbf{Z} = \mathbf{Z}_\circ\mathbf{R}_{\mathsf{QR}}$ as in (6.6), we obtain exactly as in (6.8)

$$\mathbf{r}_n = \begin{bmatrix} \mathbf{Z}_\circ & \mathbf{V}_{n+1} \end{bmatrix} \underline{\mathbf{q}}_n\,, \tag{8.4}$$

where

$$\underline{\mathbf{q}}_n :\equiv \begin{bmatrix} \mathbf{q}_n^\circ \\ \underline{\mathbf{q}}_n^\perp \end{bmatrix} :\equiv \begin{bmatrix} \mathbf{R}_{\mathsf{QR}}\widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 \\ \underline{\mathbf{e}}_1\beta \end{bmatrix} - \begin{bmatrix} \mathbf{R}_{\mathsf{QR}} & \mathbf{R}_{\mathsf{QR}}\mathbf{C}_n \\ \mathbf{O} & \underline{\mathbf{T}}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} \quad \in \mathbb{C}^{k+n+1} \tag{8.5}$$

is now the *deflated QMR quasi-residual*. Note that formally the only change is the replacement of the extended Hessenberg matrix $\underline{\mathbf{H}}_n$ by an extended tridiagonal matrix $\underline{\mathbf{T}}_n$ (or a block tridiagonal one if look-ahead steps are needed). This means short recurrences (except for the very unlikely special situation of a long look-ahead step) and thus no need to store the

[4]Except that in [32] $\mathbf{v}_k$ and $\widetilde{\mathbf{v}}_k$ were called $\mathbf{y}_k$ and $\widetilde{\mathbf{y}}_k$, respectively.

columns of $\mathbf{V}_n$ and $\widetilde{\mathbf{V}}_n$ since, in fact, the component $\mathbf{V}_n\mathbf{k}_n$ of the approximate solutions $\mathbf{x}_n$ can be updated step by step, as in MINRES.

Since we have chosen to QR-decompose $\mathbf{Z}$ — assuming that the number k of its columns is small — we still have $\|\mathbf{q}_n^\circ\|_2 = \|\mathbf{Q}\mathbf{r}_n\|_2$ as in (6.11). However, the other essential change is that the columns of $\mathbf{V}_{n+1}$ are no longer orthogonal, so, in general, $\|\underline{\mathbf{q}}_n^\perp\|_2 \neq \|\mathbf{P}\mathbf{r}_n\|_2$, unlike in (6.11). And, since $\mathbf{V}_n$ has changed, so has $\mathbf{C}_n :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{A}\mathbf{V}_n$.

Nevertheless, as in QMR, we may choose to minimize $\|\underline{\mathbf{q}}_n\|_2$ instead of $\|\mathbf{r}_n\|_2$, and as in Section 2 this amounts to solving first an $n \times (n+1)$ least squares problem with the extended tridiagonal matrix $\underline{\mathbf{T}}_n$ for minimizing $\|\mathbf{q}_n^\perp\|_2$ and for finding $\mathbf{k}_n$. Next, $\mathbf{m}_n$ is chosen such that $\mathbf{q}_n^\circ = \mathbf{o}$:

$$\min \|\underline{\mathbf{q}}_n\|_2 = \min \|\underline{\mathbf{q}}_n^\perp\|_2 = \min_{\mathbf{k}_n \in \mathbb{C}^n} \|\underline{\mathbf{e}}_1\beta - \underline{\mathbf{T}}_n\mathbf{k}_n\|_2 \,, \qquad \mathbf{m}_n := \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n \,. \tag{8.6}$$

As in Section 6, the QR decomposition of $\mathbf{Z}$ is seen to be unnecessary. Updating the least squares problem (8.6) by updating the QR decomposition of $\underline{\mathbf{T}}_n$ is done as in MINRES and QMR.

Also deflated QMR can break down in the same way as deflated GMRES. The corresponding adaptation of the first part of Theorem 2 again requires only minor changes. But additionally, QMR may break down due to a serious breakdown of the nonsymmetric Lanczos process; see, *e.g.*, [26, 32] for a discussion of these breakdowns. They can nearly always be circumnavigated by look-ahead.

THEOREM 11. *If $\widehat{\mathbf{r}}_0 \notin \mathcal{N}(\widehat{\mathbf{A}})$, then as long as $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n = \{\mathbf{o}\}$ and as long as there are no serious Lanczos breakdowns, the deflated QMR method defined by (6.5) and (8.3)–(8.6) yields in the nth step the approximate solution $\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ whose quasi-residual $\underline{\mathbf{q}}_n$ defined by (8.5) has minimal 2-norm.*

However, apart from Lanczos breakdowns, if $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widetilde{\mathcal{Z}}^\perp \neq \{\mathbf{o}\}$ and if $\mathbf{x}_0$ is chosen such that $\widehat{\mathbf{r}}_0 \in \mathcal{N}(\widehat{\mathbf{A}})$, then (and only then) deflated QMR breaks down in the first step where $n = 1$. Moreover, at step $n > 1$, if (and only if) $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_n \neq \{\mathbf{o}\}$, the method breaks down when attempting to construct $\mathbf{v}_n$. In case of these two latter types of breakdown, the search space $\mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$ does not contain the exact solution.

Proof. Here, we have to replace in the proof of Theorem 2 not only every occurrence of $\mathcal{Z}^\perp$ by $\widetilde{\mathcal{Z}}^\perp$, but also $\mathbf{V}_n^{\mathsf{H}}$ by $\widetilde{\mathbf{V}}_n^{\mathsf{H}}$, $\underline{\mathbf{H}}_n$ by $\underline{\mathbf{T}}_n$, 'orthogonality to $\widehat{\mathcal{K}}_n$' by 'orthogonality to $\widehat{\mathcal{L}}_n$', and 'Arnoldi' by 'Lanczos'. Then the arguments remain the same as in the proof of Theorem 9. □

9. Deflation by oblique projection: deflated simplified QMR. If $\mathbf{A}$ is Hermitian and the Lanczos biorthogonalization algorithm is started with $\widetilde{\mathbf{v}}_0 = \mathbf{v}_0$, then it simplifies to the symmetric Lanczos algorithm since $\widetilde{\mathbf{V}}_n = \mathbf{V}_n$ and $\widetilde{\mathbf{T}}_n = \overline{\mathbf{T}_n} = \mathbf{T}_n$. Consequently, QMR just simplifies to MINRES, where, in particular, only one matrix-vector product is needed per step. As pointed out by Freund [25] there are other situations where one can profit from a similar simplification. In fact, Rutishauser [50] made the point that, in theory, the matrix-vector product by $\mathbf{A}^{\mathsf{H}}$ in the nonsymmetric Lanczos algorithm can be avoided since, for every square matrix $\mathbf{A}$ there exists a nonsingular matrix $\mathbf{S}$ such that $\mathbf{A}^{\mathsf{T}} = \mathbf{S}\mathbf{A}\mathbf{S}^{-1}$, that is, $\mathbf{A}^{\mathsf{T}}$ is always similar to $\mathbf{A}$; see, *e.g.*, [35, p. 134] for a proof of this result. Choosing $\widetilde{\mathbf{v}}_0 = \overline{\mathbf{S}\mathbf{v}_0}$ yields then $\widetilde{\mathbf{v}}_n = \overline{\mathbf{S}\mathbf{v}_n}$ for $n > 0$; therefore, the multiplication by $\mathbf{A}^{\mathsf{H}}$ can be replaced by a multiplication by $\mathbf{S}$ followed by complex conjugation. The vectors $\widetilde{\mathbf{v}}_n$ are temporarily needed to compute the recursion coefficients stored in $\mathbf{T}_n$.

However, in general, the spectral decomposition of $\mathbf{A}$ is needed to construct $\mathbf{S}$, and this makes this idea normally unfeasible. But there are some interesting situations, where the matrix $\mathbf{S}$ is known and simple to multiply with. Freund [25] lists several classes of $\mathbf{S}$-*symmetric* and $\mathbf{S}$-*Hermitian* matrices satisfying by definition $\mathbf{A}^\mathsf{T}\mathbf{S} = \mathbf{S}\mathbf{A}$, $\mathbf{S} = \mathbf{S}^\mathsf{T}$ and $\mathbf{A}^\mathsf{H}\mathbf{S} = \mathbf{S}\mathbf{A}$, $\mathbf{S} = \mathbf{S}^\mathsf{H}$, respectively. But we note that the symmetry conditions $\mathbf{S} = \mathbf{S}^\mathsf{T}$ or $\mathbf{S} = \mathbf{S}^\mathsf{H}$ are not needed for the simplification.

In one popular application of deflated Krylov space methods, the Wilson formulation of the lattice Dirac operator in lattice Quantum Chromodynamics (QCD), the Wilson matrix $\mathbf{A}$ has the form $\mathbf{A} = \mathbf{I} - \kappa\mathbf{W}$, where $\kappa \in \mathbb{R}$ and $\mathbf{W}$ is $\mathbf{S}$-Hermitian for a diagonal matrix $\mathbf{S}$ with diagonal elements ± 1. See [7, 10, 29] for early contributions making use of this feature and [2, 1, 46, 57] for some samples of the many publications that make use of deflation in lattice QCD.

So, compared to QMR, simplified QMR reduces the cost in both time and memory. Regarding modifications for the deflated version, there is not much change before one gets to the details of an implementation. In particular, (8.4)–(8.6) remain unchanged.

10. An alternative interpretation of the augmentation component. We have seen that in each of the deflated Krylov space methods presented here and based on the ansatz $\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n + \mathbf{U}\mathbf{m}_n$, the solution can be found in two steps: first, an $(n+1)\times n$ least-square problem with an extended Hessenberg or tridiagonal matrix is solved for $\mathbf{k}_n$, then an explicit formula for $\mathbf{m}_n$ is evaluated in order to determine the augmentation component $\mathbf{U}\mathbf{m}_n$ of the approximate solution and the corresponding augmentation component $-\mathbf{Z}\mathbf{m}_n$ of the residual. As mentioned, the first part can be viewed as applying the corresponding standard Krylov space method to the singular linear system $\widehat{\mathbf{A}}\widehat{\mathbf{x}} = \widehat{\mathbf{r}}_0$. For example, in deflated GMRES, checking the derivation of the least-square problem in (2.12),

$$\min \|\mathbf{q}_n\|_2 = \min_{\mathbf{k}_n \in \mathbb{C}^n} \|\underline{\mathbf{e}}_1\beta - \underline{\mathbf{H}}_n\mathbf{k}_n\|_2 \ ,$$

we readily see that it is the coordinate space equivalent of the least squares problem

$$\|\mathbf{V}_{n+1}(\underline{\mathbf{e}}_1\beta - \underline{\mathbf{H}}_n\mathbf{k}_n)\|_2 = \|\widehat{\mathbf{r}}_0 - \mathbf{P}\mathbf{A}\mathbf{V}_n\mathbf{k}_n\|_2 = \|\widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}\mathbf{V}_n\mathbf{k}_n\|_2 = \min! \tag{10.1}$$

in the space $\mathcal{Z}^\perp$. On the other hand, $\mathbf{m}_n := \mathbf{Z}^\mathsf{H}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n$ yields in residual space

$$\mathbf{Z}\mathbf{m}_n = \mathbf{Z}\mathbf{Z}^\mathsf{H}\mathbf{r}_0 - \mathbf{Z}\mathbf{C}_n\mathbf{k}_n = \mathbf{Q}\mathbf{r}_0 - \mathbf{Q}\mathbf{A}\mathbf{V}_n\mathbf{k}_n \ , \tag{10.2}$$

a formula relating three vectors in $\mathcal{Z}$. The corresponding correction for the iterates is

$$\mathbf{U}\mathbf{m}_n = \mathbf{U}\mathbf{Z}^\mathsf{H}\mathbf{r}_0 - \mathbf{U}\mathbf{C}_n\mathbf{k}_n = \mathbf{U}\mathbf{Z}^\mathsf{H}\mathbf{b} - \mathbf{U}\mathbf{Z}^\mathsf{H}\mathbf{A}(\mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n) \, . \tag{10.3}$$

Now, let us define, with the optimal $\mathbf{k}_n$,

$$\widehat{\mathbf{x}}_n :\equiv \mathbf{V}_n\mathbf{k}_n \ , \qquad \widetilde{\mathbf{x}}_n :\equiv \mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n = \mathbf{x}_0 + \widehat{\mathbf{x}}_n \ ,$$

so that $\mathbf{x}_n = \mathbf{x}_0 + \widehat{\mathbf{x}}_n + \mathbf{U}\mathbf{m}_n = \widetilde{\mathbf{x}}_n + \mathbf{U}\mathbf{m}_n$. Then (10.1)–(10.3) take the form

$$\left\|\widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}\widehat{\mathbf{x}}_n\right\|_2 = \min_{\widehat{\mathbf{x}} \in \widehat{\mathcal{K}}_n} \left\|\widehat{\mathbf{r}}_0 - \widehat{\mathbf{A}}\widehat{\mathbf{x}}\right\|_2 \ , \tag{10.4}$$

$$\|\mathbf{P}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n)\|_2 = \min_{\widetilde{\mathbf{x}} \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n} \|\mathbf{P}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}})\|_2 \ , \tag{10.5}$$

$$\mathbf{Z}\mathbf{m}_n = \mathbf{Q}(\mathbf{r}_0 - \mathbf{A}\widehat{\mathbf{x}}_n) = \mathbf{Q}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) \, , \tag{10.6}$$

$$\mathbf{U}\mathbf{m}_n = \mathbf{U}\mathbf{Z}^\mathsf{H}(\mathbf{r}_0 - \mathbf{A}\widehat{\mathbf{x}}_n) = \mathbf{U}\mathbf{Z}^\mathsf{H}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) \, . \tag{10.7}$$

This clarifies for deflated GMRES the relationship between the problems in coordinate space and those in the Krylov subspace $\widehat{\mathcal{K}}_n \subseteq \mathcal{Z}^\perp$, in the affine space $\mathbf{x}_0 + \widehat{\mathcal{K}}_n \subseteq \mathbf{x}_0 + \mathcal{Z}^\perp$, and in the augmented space $\mathbf{x}_0 + \widehat{\mathcal{K}}_n + \mathcal{U}$.

Likewise, with differently defined matrices $\mathbf{V}_{n+1}$, $\underline{\mathbf{H}}_n$, $\mathbf{Q}$, $\mathbf{P}$, $\mathbf{C}_n$, and the new matrix $\widetilde{\mathbf{Z}}$, and thus also with different $\widehat{\mathbf{A}}$, $\widehat{\mathbf{r}}_0$, and $\widehat{\mathcal{K}}_n$, the least squares problem of truly deflated GMRES in (6.12) corresponds to one in $\widetilde{\mathcal{Z}}^\perp$ that is formally identical with (10.1) and can be recast as (10.4) or (10.5). Moreover, the formula $\mathbf{m}_n := \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n$ yields in the residual space still (10.6), while in the search space of the approximants we get analogously to (10.7)

$$\mathbf{U}\mathbf{m}_n = \mathbf{U}\widetilde{\mathbf{Z}}^{\mathsf{H}}(\mathbf{r}_0 - \mathbf{A}\widehat{\mathbf{x}}_n) = \mathbf{U}\widetilde{\mathbf{Z}}^{\mathsf{H}}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n)\,. \tag{10.8}$$

The property that (10.4) and (10.5) remain valid can be understood from the fact that in (6.11) the term $\|\mathbf{q}_n^\circ\| = \|\mathbf{Q}\mathbf{r}_n\|$ vanishes for the optimal choice of $\mathbf{x}_n$, while for the other term $\|\underline{\mathbf{q}}_n^\perp\| = \|\mathbf{P}\mathbf{r}_n\|$ the coordinate map is still isometric because the basis of $\widehat{\mathcal{K}}_{n+1}$, which consists of the columns of $\mathbf{V}_{n+1}$, is orthonormal. But, in general, even if $\widetilde{\mathcal{Z}}^\perp$ is $\mathbf{A}$–invariant, $\mathbf{r}_n$ is no longer the minimal residual from $\mathbf{r}_0 + \mathbf{A}\widehat{\mathcal{K}}_n + \mathcal{Z}$, since $\mathcal{Z}$ and $\widehat{\mathcal{K}}_n \subseteq \widetilde{\mathcal{Z}}^\perp$ need not be orthogonal to each other.

For deflated QMR, the restricted minimal norm properties (10.4) – (10.5) are no longer valid, but the derivations of (10.6) and (10.8) remain unchanged, although the matrices $\mathbf{V}_{n+1}$, $\underline{\mathbf{T}}_n$, and $\mathbf{C}_n$ have again new meanings.

Yet another interpretation of the augmentation component $\mathbf{U}\mathbf{m}_n$ is found as follows. Let us consider the oblique projection framework of Sections 5–8 first, with $\mathbf{E} :\equiv \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{Z} = \mathbf{I}_k$ as in our presentation of truly deflated GMRES and deflated QMR. We further define

$$\mathbf{M}_{\mathbf{A}} :\equiv \mathbf{U}\widetilde{\mathbf{Z}}^{\mathsf{H}}\,, \qquad \mathbf{Q}_{\mathbf{A}} :\equiv \mathbf{I} - \mathbf{M}_{\mathbf{A}}\mathbf{A} = \mathbf{I} - \mathbf{U}\widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{A}\,, \tag{10.9}$$

noting that both $\mathbf{M}_{\mathbf{A}}\mathbf{A}$ and $\mathbf{Q}_{\mathbf{A}}$ are projections. Inserting them into (10.8) we obtain

$$\mathbf{U}\mathbf{m}_n = \mathbf{M}_{\mathbf{A}}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n) = \mathbf{M}_{\mathbf{A}}\mathbf{b} - (\mathbf{I} - \mathbf{Q}_{\mathbf{A}})\widetilde{\mathbf{x}}_n\,,$$

and we end up with

$$\mathbf{x}_n = \widetilde{\mathbf{x}}_n + \mathbf{U}\mathbf{m}_n = \widetilde{\mathbf{x}}_n + \mathbf{M}_{\mathbf{A}}\mathbf{b} - (\mathbf{I} - \mathbf{Q}_{\mathbf{A}})\widetilde{\mathbf{x}}_n = \mathbf{Q}_{\mathbf{A}}\widetilde{\mathbf{x}}_n + \mathbf{M}_{\mathbf{A}}\mathbf{b}\,. \tag{10.10}$$

This formula holds for truly deflated GMRES and for deflated QMR. An analogous formula holds in the situation of Sections 2–4, that is, for GMRES and MINRES deflated with orthogonal projections. We have to replace $\widetilde{\mathbf{Z}}$ by $\mathbf{Z}$ and the pair $\mathbf{M}_{\mathbf{A}}$, $\mathbf{Q}_{\mathbf{A}}$ by

$$\mathbf{M}_{\mathbf{A}^{\mathsf{H}}} :\equiv \mathbf{U}\mathbf{Z}^{\mathsf{H}}\,, \qquad \mathbf{Q}_{\mathbf{A}^{\mathsf{H}}} :\equiv \mathbf{I} - \mathbf{M}_{\mathbf{A}^{\mathsf{H}}}\mathbf{A} = \mathbf{I} - \mathbf{U}\mathbf{Z}^{\mathsf{H}}\mathbf{A} \tag{10.11}$$

to obtain likewise

$$\mathbf{x}_n = \widetilde{\mathbf{x}}_n + \mathbf{U}\mathbf{m}_n = \mathbf{Q}_{\mathbf{A}^{\mathsf{H}}}\widetilde{\mathbf{x}}_n + \mathbf{M}_{\mathbf{A}^{\mathsf{H}}}\mathbf{b}\,. \tag{10.12}$$

The last formula is the ‘correction formula’ of Theorem 2.2 in [31] for the case where $\mathbf{B} = \mathbf{A}$ there and our normalization $\mathbf{E} = \mathbf{I}_k$ holds. Both (10.10) and (10.12) relate the approximate solutions $\mathbf{x}_n$ of the augmented and deflated method to the approximate solutions $\widetilde{\mathbf{x}}_n$ of a deflated but not augmented method: $\widetilde{\mathbf{x}}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n$. The term $\mathbf{U}\mathbf{m}_n = \mathbf{M}_{\mathbf{A}}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n)$ or $\mathbf{U}\mathbf{m}_n = \mathbf{M}_{\mathbf{A}^{\mathsf{H}}}(\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}_n)$, respectively, is the ‘correction’ due to augmentation.

11. Other projections used in augmentation and deflation methods. Many publications on particular augmentation and deflation methods apply projections that are different from the projections $\mathbf{P}$ that are the basis of our approach. In this section we introduce two parameter-dependant projections $\mathbf{P}_{\mathbf{B}}$ and $\mathbf{Q}_{\mathbf{B}}$ that cover many of published proposals, the parameter $\mathbf{B}$ being a nonsingular matrix of the same size as $\mathbf{A}$. The most relevant choices for $\mathbf{B}$ are

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	definition	null space	range	range if $\mathbf{B}=\mathbf{A}$
$\mathbf{P_B}$	$\mathbf{I}-\mathbf{AMB}$	$\mathcal{Z}$	$(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$\widetilde{\mathcal{Z}}^{\perp}$
$\mathbf{Q_B}$	$\mathbf{I}-\mathbf{MBA}$	$\mathcal{U}$	$(\mathbf{A}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$(\mathbf{A}^{\mathsf{H}}\widetilde{\mathcal{Z}})^{\perp}$
$\widehat{\mathbf{A}}_{\mathbf{B}}$	$\mathbf{P_B A}=\mathbf{P_B A Q_B}=\mathbf{AQ_B}$	$\mathcal{U}$	$(\mathbf{B}^{\mathsf{H}}\widetilde{\mathcal{U}})^{\perp}$	$\widetilde{\mathcal{Z}}^{\perp}$

TABLE 11.1
The projections $\mathbf{P_B}$ and $\mathbf{Q_B}$ and the projected operator $\widehat{\mathbf{A}}_{\mathbf{B}}$ for a generalization of the situation of Sections 5–8 .

1. $\mathbf{B}=\mathbf{I}$ for deflated CG, BiCG, and FOM [51],
2. $\mathbf{B}=\mathbf{A}^{\mathsf{H}}$ for deflated CR, GCR [17], MinRes, and GMRes,
3. $\mathbf{B}=\mathbf{A}$ for deflated BiCR [56].

We start here from a setting suitable for deflated BiCG and BiCR that will be treated fully in [30]. Then we specialize it to the setting for CG, FOM, CR, GCR, MinRes, and GMRes considered in [31], which covers most of the published approaches.

Similar to the situation in our Sections 5–8 we let

$$\mathcal{U}:\equiv\mathcal{R}(\mathbf{U}),\qquad \mathbf{Z}:\equiv\mathbf{AU},\qquad \mathcal{Z}:\equiv\mathcal{R}(\mathbf{Z}),$$
$$\widetilde{\mathcal{U}}:\equiv\mathcal{R}(\widetilde{\mathbf{U}}),\qquad \widetilde{\mathbf{Z}}:\equiv\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{U}},\qquad \widetilde{\mathcal{Z}}:\equiv\mathcal{R}(\widetilde{\mathbf{Z}}),$$

but now we exchange $\mathbf{E}$ by a more general $\mathbf{E_B}\in\mathbb{C}^{k\times k}$ and introduce a matrix $\mathbf{M}\in\mathbb{C}^{N\times N}$ that replaces our $\mathbf{Q}$:

$$\mathbf{E_B}:\equiv\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{BAU},\qquad \mathbf{M}:\equiv\mathbf{U}\mathbf{E}_{\mathbf{B}}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}.$$

Of course, we assume that $\mathbf{E_B}$ is nonsingular. Finally, we introduce two projections $\mathbf{P_B}$ and $\mathbf{Q_B}$ as well as a corresponding projection $\widehat{\mathbf{A}}_{\mathbf{B}}$ of $\mathbf{A}$, all defined in Table 11.1, which also lists kernels and ranges of these three operators. In the case where $\mathbf{B}=\mathbf{I}$ these operators have been used by Erlangga and Nabben [20].

In contrast, by comparing $\mathbf{E_B}$ with $\mathbf{E}$ we see that in Section 5 the choice was $\mathbf{B}=\mathbf{A}$. In this case we have

$$\mathbf{E_A}=\mathbf{E},\quad \mathbf{AMA}=\mathbf{ZE}^{-1}\widetilde{\mathbf{Z}}^{\mathsf{H}}=\mathbf{Q},\quad \mathbf{P_A}=\mathbf{P},\quad \mathbf{Q_A}=\mathbf{I}-\mathbf{MA}^2,\quad \widehat{\mathbf{A}}_{\mathbf{A}}=\mathbf{PA}.$$

Note that $\mathbf{Q_A}$ is the same as in (10.9) if $\mathbf{E}=\mathbf{I}_k$ since $\mathbf{MA}=\mathbf{UE}_{\mathbf{A}}^{-1}\widetilde{\mathbf{U}}^{\mathsf{H}}\mathbf{A}=\mathbf{UE}^{-1}\widetilde{\mathbf{Z}}^{\mathsf{H}}=\mathbf{U}\widetilde{\mathbf{Z}}^{\mathsf{H}}=\mathbf{M_A}$. However, $\widehat{\mathbf{A}}\neq\widehat{\mathbf{A}}_{\mathbf{A}}$ in general. But the following holds:

THEOREM 12. *For the projected operators $\widehat{\mathbf{A}}$ of Sections 5–8 and $\widehat{\mathbf{A}}_{\mathbf{B}}$ of Table 11.1 with $\mathbf{B}=\mathbf{A}$ holds*

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}}=\mathbf{O}\big|_{\mathcal{Z}},\qquad \widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\widehat{\mathbf{A}}_{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}. \tag{11.1}$$

Moreover, under the assumptions of Theorem 7, where $\mathcal{Z}\oplus\widetilde{\mathcal{Z}}^{\perp}=\mathbb{C}^N$,

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}}=\widehat{\mathbf{A}}_{\mathbf{A}}\big|_{\mathcal{Z}}=\mathbf{O}\big|_{\mathcal{Z}},\qquad \widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\widehat{\mathbf{A}}_{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\mathbf{A}\big|_{\widetilde{\mathcal{Z}}^{\perp}}, \tag{11.2}$$

and therefore $\widehat{\mathbf{A}}=\widehat{\mathbf{A}}_{\mathbf{A}}$ on $\mathbb{C}^N$.

Proof. By definition, $\widehat{\mathbf{A}}=\mathbf{PAP}$, where $\mathbf{P}$ is a projection with $\mathcal{N}(\mathbf{P})=\mathcal{Z}$ and $\mathcal{R}(\mathbf{P})=\widetilde{\mathcal{Z}}^{\perp}$. Consequently, $\widehat{\mathbf{A}}\big|_{\mathcal{Z}}=\mathbf{O}\big|_{\mathcal{Z}}$ and

$$\widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\mathbf{PAP}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\mathbf{PA}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\mathbf{P_A A}\big|_{\widetilde{\mathcal{Z}}^{\perp}}=\widehat{\mathbf{A}}_{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}}.$$

	definition	null space	range	range if $\mathbf{B} = \mathbf{A}^{\mathsf{H}}$
$\mathbf{P_B}$	$\mathbf{I} - \mathbf{AMB}$	$\mathcal{Z}$	$(\mathbf{B}^{\mathsf{H}}\mathcal{U})^{\perp}$	$\mathcal{Z}^{\perp}$
$\mathbf{Q_B}$	$\mathbf{I} - \mathbf{MBA}$	$\mathcal{U}$	$(\mathbf{A}^{\mathsf{H}}\mathbf{B}^{\mathsf{H}}\mathcal{U})^{\perp}$	$(\mathbf{A}^{\mathsf{H}}\mathcal{Z})^{\perp}$
$\widehat{\mathbf{A}}_{\mathbf{B}}$	$\mathbf{P_B A} = \mathbf{P_B A Q_B} = \mathbf{A Q_B}$	$\mathcal{U}$	$(\mathbf{B}^{\mathsf{H}}\mathcal{U})^{\perp}$	$\mathcal{Z}^{\perp}$

TABLE 11.2
The projections $\mathbf{P_B}$ and $\mathbf{Q_B}$ and the projected operator $\widehat{\mathbf{A}}_{\mathbf{B}}$ for a generalization of the situation of Sections 2–4.

Moreover, if $\mathcal{Z}$ is $\mathbf{A}$–invariant,

$$\widehat{\mathbf{A}}_{\mathbf{A}}\mathcal{Z} = \mathbf{PA}\mathcal{Z} \subseteq \mathbf{P}\mathcal{Z} = \{\mathbf{o}\}.$$

Finally, under the assumptions of Theorem 7, also $\widetilde{\mathcal{Z}}^{\perp}$ is $\mathbf{A}$–invariant and, by (5.6),

$$\widehat{\mathbf{A}}\big|_{\widetilde{\mathcal{Z}}^{\perp}} = \mathbf{A}\big|_{\widetilde{\mathcal{Z}}^{\perp}}.$$

Altogether, we obtain (11.2) and, since $\mathcal{Z} \oplus \widetilde{\mathcal{Z}}^{\perp} = \mathbb{C}^N$ under these assumptions, there holds $\widehat{\mathbf{A}} = \widehat{\mathbf{A}}_{\mathbf{A}}$ on $\mathbb{C}^N$. □

An analogous result holds in the situation of Sections 2–4. There is no dual space there, so we redefine

$$\mathbf{E_B} :\equiv \mathbf{U}^{\mathsf{H}}\mathbf{BAU}, \qquad \mathbf{M} :\equiv \mathbf{U}\mathbf{E}_{\mathbf{B}}^{-1}\mathbf{U}^{\mathsf{H}}.$$

$\mathbf{P_B}$, $\mathbf{Q_B}$, and $\widehat{\mathbf{A}}_{\mathbf{B}}$ can be defined as before, but their ranges slightly differ; see Table 11.2. This is the situations considered in [31]. (But note that our $\mathbf{B}$ is defined differently and equals $\mathbf{B}^{\mathsf{H}}$ in the notation of [31].) The case where $\mathbf{B} = \mathbf{I}$ covers deflated CG [48, 13, 41, 61, 19, 54] and is also a topic of study in [21, 47, 60] and related work.

Comparing $\mathbf{E_B}$ with $\mathbf{E}$ of Section 2 we see that $\mathbf{B} = \mathbf{A}^{\mathsf{H}}$ here. Then we have

$$\mathbf{E}_{\mathbf{A}^{\mathsf{H}}} = \mathbf{E}, \quad \mathbf{AMA}^{\mathsf{H}} = \mathbf{ZE}^{-1}\mathbf{Z}^{\mathsf{H}} = \mathbf{Q}, \quad \mathbf{P}_{\mathbf{A}^{\mathsf{H}}} = \mathbf{P}, \quad \mathbf{Q}_{\mathbf{A}^{\mathsf{H}}} = \mathbf{I} - \mathbf{MA}^{\mathsf{H}}\mathbf{A}, \quad \widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}} = \mathbf{PA}.$$

Now $\mathbf{Q}_{\mathbf{A}^{\mathsf{H}}}$ is the same as in (10.11) if $\mathbf{E} = \mathbf{I}_k$ since $\mathbf{MA}^{\mathsf{H}} = \mathbf{UE}_{\mathbf{A}^{\mathsf{H}}}^{-1}\mathbf{U}^{\mathsf{H}}\mathbf{A}^{\mathsf{H}} = \mathbf{UE}^{-1}\mathbf{Z}^{\mathsf{H}} = \mathbf{UZ}^{\mathsf{H}} = \mathbf{M}_{\mathbf{A}^{\mathsf{H}}}$. The following analog of Theorem 12 holds:

THEOREM 13. *For the projected operators $\widehat{\mathbf{A}}$ of Sections 2–4 and $\widehat{\mathbf{A}}_{\mathbf{B}}$ of Table 11.2 with $\mathbf{B} = \mathbf{A}^{\mathsf{H}}$ holds*

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}} = \mathbf{O}\big|_{\mathcal{Z}}, \qquad \widehat{\mathbf{A}}\big|_{\mathcal{Z}^{\perp}} = \widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}}\big|_{\mathcal{Z}^{\perp}}. \tag{11.3}$$

Moreover, if $\mathcal{Z}$ and $\mathcal{Z}^{\perp}$ are $\mathbf{A}$–invariant, then

$$\widehat{\mathbf{A}}\big|_{\mathcal{Z}} = \widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}}\big|_{\mathcal{Z}} = \mathbf{O}\big|_{\mathcal{Z}}, \qquad \widehat{\mathbf{A}}\big|_{\mathcal{Z}^{\perp}} = \widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}}\big|_{\mathcal{Z}^{\perp}} = \mathbf{A}\big|_{\mathcal{Z}^{\perp}}, \tag{11.4}$$

and therefore $\widehat{\mathbf{A}} = \widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}}$ on $\mathbb{C}^N$.

Proof. The proof is fully analogous to the one of Theorem 12 and is left out here. □

In summary, the two slightly different projections $\mathbf{P}$ used here in Sections 2–4 and in Sections 5–8 coincide with the projections $\mathbf{P}_{\mathbf{A}^{\mathsf{H}}}$ and $\mathbf{P_A}$ defined in Table 11.2 (for $\mathbf{B} = \mathbf{A}^{\mathsf{H}}$) and Table 11.1 (for $\mathbf{B} = \mathbf{A}$), respectively, but they differ from the projections $\mathbf{P_I}$ defined there when $\mathbf{B} = \mathbf{I}$. The latter projections are those used in deflated CG [48, 13, 41] and deflated BICG [30]. Moreover, even when $\mathbf{P} = \mathbf{P}_{\mathbf{A}^{\mathsf{H}}}$ or $\mathbf{P} = \mathbf{P_A}$ our deflated operator $\widehat{\mathbf{A}} = \mathbf{PAP}$ differs in general from the deflated operators $\widehat{\mathbf{A}}_{\mathbf{A}^{\mathsf{H}}}$ and $\widehat{\mathbf{A}}_{\mathbf{A}}$, respectively, unless $\mathcal{Z}$ and $\mathcal{Z}^{\perp}$ or $\widetilde{\mathcal{Z}}^{\perp}$ are exactly right and left $\mathbf{A}$–invariant subspaces.

12. Deflated quasi-(bi)orthogonal residual methods. The GMRES algorithm of Saad and Schultz [53] is just one incidence of a so-called minimal residual (MR) method: a Krylov space solver whose iterates and residuals restricted by

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,, \qquad \mathbf{r}_n \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0) \tag{12.1}$$

have the minimal norm property $\|\mathbf{r}_n\|_2 = \min!$, which is equivalent to the Galerkin condition

$$\mathbf{r}_n \perp \mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,. \tag{12.2}$$

Other methods with the same mathematical properties are the Generalized Minimum Residual (GCR) method [17], the MINRES algorithm of Paige and Saunders [49] for Hermitian matrices, and, the Conjugate Residual (CR) method of Stiefel [59] for Hpd matrices. While MINRES and GMRES transplant the problem into coordinate space, CG and GCR use directly recursions for $\mathbf{x}_n$ and $\mathbf{r}_n$.

There is an analogue family of so-called orthogonal residual (OR) methods, where (12.2) is replaced by another Galerkin condition,

$$\mathbf{r}_n \perp \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)\,, \tag{12.3}$$

which implies that the residuals are mutually orthogonal. This family includes the ubiquitous conjugate gradient (CG) method of Hestenes and Stiefel [34] for Hpd matrices, which has the property that the residuals have minimal $\mathbf{A}^{-1}$–norm, or, equivalently, the error vectors have minimal $\mathbf{A}$–norm. Another one is the Full Orthogonalization Method (FOM) of Saad [51]. Of course, if $\mathbf{A}$ is not Hpd, there is no $\mathbf{A}^{-1}$–norm, and therefore no minimal norm property. Moreover, for some n an iterate characterized by (12.1) and (12.3) need not exist. Therefore there is little interest in this method.

Of much greater importance is the biconjugate gradient (BICG) method of Lanczos [40] and Fletcher [23], where the Galerkin condition (12.3) is replaced by the Petrov-Galerkin condition

$$\mathbf{r}_n \perp \mathcal{K}_n(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{r}}_0)\,, \tag{12.4}$$

with a freely selectable $\widetilde{\mathbf{r}}_0$. There is still the drawback that iterates may not exist and further breakdown problems lurk (see, *e.g.*, [32]), but this is balanced by the enormous advantage of short recurrences for iterates and residuals. Eq. (12.4) implies that the residuals $\mathbf{r}_n$ and the so-called shadow residuals $\widetilde{\mathbf{r}}_n$ of the fictitious linear system $\mathbf{A}^{\mathsf{H}}\widetilde{\mathbf{x}} = \widetilde{\mathbf{r}}_0$ (with initial approximation $\widetilde{\mathbf{x}}_0 := \mathbf{o}$) are mutually biorthogonal.

If we consider a transplantation of an OR method to coordinate space, it follows immediately that $\mathbf{r}_n = \mathbf{r}_0 + \mathbf{A}\mathbf{V}_n\mathbf{k}_n$ is a scalar multiple of $\mathbf{v}_n$, the $(n+1)$th basis vector generated by the Arnoldi or the nonsymmetric Lanczos process, respectively. Moreover, inserting the Arnoldi relation $\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{H}}_n$ or the Lanczos relation $\mathbf{A}\mathbf{V}_n = \mathbf{V}_{n+1}\underline{\mathbf{T}}_n$ we see that the coordinate vector $\mathbf{k}_n$ satisfies

$$\mathbf{H}_n\mathbf{k}_n = \mathbf{e}_1\beta \qquad \text{or} \qquad \mathbf{T}_n\mathbf{k}_n = \mathbf{e}_1\beta\,, \tag{12.5}$$

respectively, with the $n \times n$ matrices $\mathbf{H}_n$ and $\mathbf{T}_n$ that are the 'upper parts' of the matrices $\underline{\mathbf{H}}_n$ and $\underline{\mathbf{T}}_n$ used in the coordinate space based MR methods. Solving recursively these linear systems by LR or QR factorization we obtain coordinate based OR methods. In the case of the tridiagonal matrices $\mathbf{T}_n$ it is possible to derive short recurrences for the iterates and residuals, but this means essentially that we apply a CG-like or BICG-like algorithm.

In this section we want to point out that we can define augmented and deflated methods that are not quite (bi)orthogonal residual methods, but might be called *deflated quasi-(bi)orthogonal residual methods* and have the property that they turn into *deflated (bi)orthogonal residual methods* if $\mathcal{K}$ is $\mathbf{A}$–invariant. We start again from

$$\mathbf{x}_n = \mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n + \mathbf{U}\mathbf{m}_n\,, \qquad \mathbf{r}_n = \mathbf{r}_0 - \mathbf{A}\mathbf{V}_n\mathbf{k}_n - \mathbf{Z}\mathbf{m}_n\,. \tag{12.6}$$

and a representation of $\mathbf{r}_n$ in terms of the basis of $\mathcal{K}_{n+1} \oplus \mathcal{Z}$ given by $\begin{bmatrix} \mathbf{V}_{n+1} & \mathbf{Z} \end{bmatrix}$. Deflated CG [48, 13, 41, 61, 19, 54] and deflated FOM are normally characterized by

$$\mathbf{r}_n \perp \widehat{\mathcal{K}}_n \oplus \mathcal{U}\,. \tag{12.7}$$

For CG, *i.e.*, for Hpd $\mathbf{A}$, it has been implicitly shown in various ways [13, 36, 48] (see also [19, Thm. 4.1] and [54, Thm 4.2]) that this implies the following optimality result, for which we provide the sketch of a straightforward proof.

THEOREM 14. *Assume $\mathbf{A}$ is Hpd, define $\mathcal{K}_n$ and $\mathcal{U}$ as in Section 2, and let again $\mathbf{x}_\star :\equiv \mathbf{A}^{-1}\mathbf{b}$. Then the condition (12.7) implies that $\mathbf{x}_n$ is optimal in the sense that $\|\mathbf{x}_n - \mathbf{x}_\star\|_{\mathbf{A}}$ is minimal under the restriction $\mathbf{x}_n \in \mathbf{x}_0 + \widehat{\mathcal{K}}_n \oplus \mathcal{U}$.*

Proof. Assume $\mathbf{x}_n$ and $\mathbf{r}_n$ are represented as in (12.6), and let

$$\Psi(\mathbf{k}_n, \mathbf{m}_n) :\equiv \tfrac{1}{2}\,\|\mathbf{x}_n - \mathbf{x}_\star\|^2_{\mathbf{A}} = \tfrac{1}{2}\,\|\mathbf{x}_0 + \mathbf{V}_n\mathbf{k}_n + \mathbf{U}\mathbf{m}_n - \mathbf{x}_\star\|^2_{\mathbf{A}}\,.$$

Then straightforward differentiation shows that

$$\frac{\partial\Psi}{\partial\mathbf{k}_n} = -\,\mathbf{r}_n^{\mathsf{H}}\mathbf{V}_n\,, \qquad \frac{\partial\Psi}{\partial\mathbf{m}_n} = -\,\mathbf{r}_n^{\mathsf{H}}\mathbf{U}\,,$$

and

$$\frac{\partial^2\Psi}{(\partial\mathbf{k}_n)^2} = \mathbf{V}_n^{\mathsf{H}}\mathbf{A}\mathbf{V}_n\,, \qquad \frac{\partial^2\Psi}{\partial\mathbf{k}_n\,\partial\mathbf{m}_n} = \mathbf{O}\,, \qquad \frac{\partial^2\Psi}{(\partial\mathbf{m}_n)^2} = \mathbf{U}^{\mathsf{H}}\mathbf{A}\mathbf{U}\,.$$

Any stationary point is characterized by zero gradients, that is, by $\mathbf{r}_n \perp \mathcal{R}(\mathbf{V}_n) = \mathcal{K}_n$ and $\mathbf{r}_n \perp \mathcal{R}(\mathbf{U}) = \mathcal{U}$. Moreover, we have there a minimum since $\mathbf{V}_n^{\mathsf{H}}\mathbf{A}\mathbf{V}_n$ and $\mathbf{U}^{\mathsf{H}}\mathbf{A}\mathbf{U}$ are Hpd. $\square$

The deflated CG algorithms of [48, 13, 41, 61, 19, 54] fulfill condition (12.7), and thus maintain global optimality. For deflation they implicitly or explicitly apply oblique projections, namely $\mathbf{P_I}$ or $\mathbf{Q_I}$ of Table 11.2 (with $\mathbf{B} = \mathbf{I}$ and $\mathbf{A}^{\mathsf{T}} = \mathbf{A}$, so that $\mathbf{P_I} = \mathbf{Q}_{\mathbf{I}}^{\mathsf{T}}$). Dostál [13] calls $\mathbf{MA}$ a *conjugate projection*. Moreover, these algorithms are all based on recurrences for iterates and residuals, so they are not coordinate space based. But unless $\mathcal{Z}$ is exactly $\mathbf{A}$–invariant, the approach promoted in this paper which leads to the decomposition $\widehat{\mathcal{K}}_n \oplus \mathcal{Z}$ is in conflict with a global optimization criteria valid for $\widehat{\mathcal{K}}_n \oplus \mathcal{U}$. To obtain simple coordinate space based methods we may drop global optimality and replace (12.7) by

$$\mathbf{r}_n \perp \widehat{\mathcal{K}}_n \oplus \mathcal{Z}\,. \tag{12.8}$$

We will call a method with this property a *deflated quasi-orthogonal residual (DQOR) method*. For such a method we have the following trivial corollary.

COROLLARY 15. *Under the assumptions of Theorem 14, if $\mathcal{Z}$ is $\mathbf{A}$–invariant, the condition (12.8) implies that $\mathbf{x}_n$ is optimal in the sense that $\|\mathbf{x}_n - \mathbf{x}_\star\|_{\mathbf{A}}$ is minimal under the restriction (12.1).*

Proof. If $\mathcal{Z}$ is $\mathbf{A}$–invariant, $\mathcal{U} = \mathbf{A}^{-1}\mathcal{Z} = \mathcal{Z}$. So, (12.8) implies (12.7) here. $\square$

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With the quasi-residual $\underline{\mathbf{q}}_n$ of (2.10), the condition (12.8) transforms into

$$\underline{\mathbf{q}}_n \perp \mathbb{C}^{k+n} \tag{12.9}$$

if we consider $\mathbb{C}^{k+n}$ as the subspace of $\mathbb{C}^{k+n+1}$ characterized by a zero last component. This means that the first $k+n$ components of $\underline{\mathbf{q}}_n$ must be zero, that is,

$$\begin{bmatrix} \mathbf{I}_k & \mathbf{C}_n \\ \mathbf{O} & \mathbf{H}_n \end{bmatrix} \begin{bmatrix} \mathbf{m}_n \\ \mathbf{k}_n \end{bmatrix} = \begin{bmatrix} \mathbf{Z}^{\mathsf{H}}\mathbf{r}_0 \\ \mathbf{e}_1\beta \end{bmatrix}. \tag{12.10}$$

This system is upper block triangular with a unit $(1,1)$ block, and therefore it reduces to a linear system with the $(2,2)$ block for computing $\mathbf{k}_n$ and an explicit formula for $\mathbf{m}_n$, in complete analogy to the least squares problem (2.11) that we solved before:

$$\mathbf{H}_n\mathbf{k}_n = \mathbf{e}_1\beta\,, \qquad \mathbf{m}_n := \mathbf{Z}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n\,. \tag{12.11}$$

In the setting of deflated GMRES of Section 2 these two formulas define a corresponding particular DQOR method. If $\mathbf{A}$ is Hermitian, we can replace $\mathbf{H}_n$ by the tridiagonal $\mathbf{T}_n$ and profit from short recurrences for updating $\mathbf{x}_n$.

In the setting of truly deflated GMRES of Section 6, where $\underline{\mathbf{q}}_n$ is defined by (6.9), the conditions (12.8) and (12.9) are no longer equivalent. For simplicity we may just fulfil the latter, which yields (12.10), except that $\mathbf{Z}^{\mathsf{H}}$ is replaced by $\widetilde{\mathbf{Z}}^{\mathsf{H}}$, so that (12.11) turns into

$$\mathbf{H}_n\mathbf{k}_n = \mathbf{e}_1\beta\,, \qquad \mathbf{m}_n := \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n\,. \tag{12.12}$$

This defines another particular DQOR method.

Finally, in the setting of deflated QMR of Section 8 condition (12.9) leads to

$$\mathbf{T}_n\mathbf{k}_n = \mathbf{e}_1\beta\,, \qquad \mathbf{m}_n := \widetilde{\mathbf{Z}}^{\mathsf{H}}\mathbf{r}_0 - \mathbf{C}_n\mathbf{k}_n\,. \tag{12.13}$$

As can be readily verified, in this setting condition (12.9) is equivalent to

$$\mathbf{r}_n \perp \widehat{\mathcal{L}}_n \oplus \widetilde{\mathcal{Z}}\,, \tag{12.14}$$

which characterizes a *deflated quasi-biorthogonal residual (*DQBIOR*) method*. The Recycling BICG (RBICG) method of Ahuja [4, 5] seems to be of this type.

DQOR and DQBIOR methods are in general not optimal. But we think that this is a minor disadvantage. It is shared by the class of orthogonal residual methods, whose residual norms depend in a well-known way discovered by Paige and Saunders [49] from those of the corresponding MR method; see, *e.g.*, [16] and [33].

Conclusions. We have described several augmented and deflated Krylov methods for solving $\mathbf{Ax} = \mathbf{b}$ that all fit into a common theoretical framework. They are coordinate space based in the sense that we generate recursively bases for the augmented search spaces $\widehat{\mathcal{K}}_n \oplus \mathcal{U}$ and $\widehat{\mathcal{K}}_{n+1} \oplus \mathcal{Z}$ for the iterates $\mathbf{x}_n$ and the corresponding residual $\mathbf{r}_n$, respectively, and determine the coordinates of $\mathbf{x}_n$. Here, $\mathcal{Z} = \mathbf{A}\mathcal{U}$. The typical examples are deflated MINRES, GMRES, and QMR. Details differ from the proposals in the literature: for MINRES a little, for GMRES much more.

We assume that a basis for $\mathcal{U}$ is given, and that typically, but not necessarily, this subspace is close to an $\mathbf{A}$–invariant subspace belonging to eigenvalues of small absolute value. Deflation replaces these by zero. We point out that the deflated operator $\widehat{\mathbf{A}} :\equiv \mathbf{PAP}$ and the corresponding Krylov subspaces $\widehat{\mathcal{K}}_n :\equiv \mathcal{K}_n(\widehat{\mathbf{A}}, \widehat{\mathbf{r}}_0)$ generated from $\widehat{\mathbf{r}}_0 :\equiv \mathbf{P}\mathbf{r}_0$ can be chosen in different ways. For deflated MINRES an orthogonal projection $\mathbf{P}$ on $\mathcal{Z}^\perp$ is appropriate. The same projection is also the standard for deflated GMRES. We suggest for non-Hermitian $\mathbf{A}$ another choice: an oblique projection onto $\widetilde{\mathcal{Z}}^\perp$ along $\mathcal{Z}$. Here $\widetilde{\mathcal{Z}}$ is an approximately left $\mathbf{A}$–invariant subspace corresponding to the same eigenvalues as $\mathcal{U}$ and $\mathcal{Z}$. This choice has the major advantage that in the case of exact $\mathbf{A}$–invariance, these eigenspaces are really deflated in the sense that the kernel of $\widehat{\mathbf{A}}$ contains $\mathcal{U} = \mathcal{Z}$, while on $\widetilde{\mathcal{Z}}^\perp$ the operators $\widehat{\mathbf{A}}$ and $\mathbf{A}$ coincide. The so deflated methods are based on the nonorthogonal decomposition $\mathcal{Z} \oplus \widehat{\mathcal{K}}_{n+1} \subseteq \mathcal{Z} \oplus \widetilde{\mathcal{Z}}^\perp = \mathbb{C}^N$, which needs to be complimented by an analogous nonorthogonal decomposition $\widetilde{\mathcal{Z}} \oplus \widehat{\mathcal{L}}_{n+1} \subseteq \widetilde{\mathcal{Z}} \oplus \mathcal{Z}^\perp = \mathbb{C}^N$ for the shadow residual search space if the nonsymmetric Lanczos algorithm is applied to generate the bases. These decompositions lead to truly deflated GMRES and deflated QMR.

As further alternatives we suggest deflated quasi-orthogonal residual (DQOR) methods and deflated quasi-biorthogonal residual (DQBIOR) methods that are simple analogs of the deflated MR and QMR methods discussed before.

While the deflated operators $\widehat{\mathbf{A}}$ we promote are defined differently from those in most of the literature (except for the one in, *e.g.*, [62], which coincides in the symmetric case), we can show that in the case where $\mathcal{Z}$ is exactly $\mathbf{A}$–invariant our deflated operators are equivalent with those (for Hermitian and non-Hermitian problems, respectively) that are discussed in two companion papers [31, 30] and have the widely used standard form, but are geared towards different Petrov-Galerkin conditions.

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Appendix: An example where deflated MINRES and GMRES break down after any given number of steps. Let us consider examples of size $N \times N$ that are of the following form:

$$\mathbf{A} := \begin{bmatrix} 0 & 1 & \mathbf{o}^\mathsf{T} \\ 1 & 0 & \mathbf{o}^\mathsf{T} \\ \mathbf{o} & \mathbf{o} & \mathbf{M} \end{bmatrix}, \qquad \mathbf{P} := \begin{bmatrix} 1 & 0 & \mathbf{o}^\mathsf{T} \\ 0 & 0 & \mathbf{o}^\mathsf{T} \\ \mathbf{o} & \mathbf{o} & \mathbf{I}_{N-2} \end{bmatrix},$$

where $\mathbf{M}$ is a symmetric nonsingular $(N-2) \times (N-2)$ matrix whose minimal polynomial is of degree κ, where $1 \leq \kappa \leq N-2$. Clearly, $\mathbf{A}$ is real symmetric and nonsingular too. We obtain

$$\mathbf{PA} = \begin{bmatrix} 0 & 1 & \mathbf{o}^\mathsf{T} \\ 0 & 0 & \mathbf{o}^\mathsf{T} \\ \mathbf{o} & \mathbf{o} & \mathbf{M} \end{bmatrix}, \qquad \widehat{\mathbf{A}} = \mathbf{PAP} = \begin{bmatrix} 0 & 0 & \mathbf{o}^\mathsf{T} \\ 0 & 0 & \mathbf{o}^\mathsf{T} \\ \mathbf{o} & \mathbf{o} & \mathbf{M} \end{bmatrix},$$

so that in the notation of Section 2 we have in particular

$$\begin{aligned} \mathcal{Z} = \mathcal{N}(\mathbf{P}) &= \mathsf{span}\,\{\mathbf{e}_2\}\,, \\ \mathcal{Z}^\perp = \mathcal{R}(\mathbf{P}) &= \mathbb{C}^N \ominus \mathsf{span}\,\{\mathbf{e}_2\}\,, \\ \mathbf{A}\mathcal{Z}^\perp = \mathcal{R}(\mathbf{AP}) &= \mathbb{C}^N \ominus \mathsf{span}\,\{\mathbf{e}_1\}\,, \\ \mathcal{N}(\widehat{\mathbf{A}}) &= \mathsf{span}\,\{\mathbf{e}_1,\, \mathbf{e}_2\}\,, \\ \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp &= \mathsf{span}\,\{\mathbf{e}_1\}\,. \end{aligned}$$

We can choose $\mathbf{b}$ and $\mathbf{x}_0$ such that $\mathbf{r}_0 = \widehat{\mathbf{r}}_0 = \mathbf{P}\mathbf{r}_0 = \begin{bmatrix} 1 & 0 & \mathbf{w}^\mathsf{T} \end{bmatrix}^\mathsf{T}$, where $\mathbf{w}$ satisfies

$$\mathbf{w} = \sum_{i=1}^{\kappa} \beta_i \, \mathbf{M}^i \, \mathbf{w} \tag{12.15}$$

with $\beta_\kappa \neq 0$. Here, $1 - \sum_{i=1}^{\kappa} \beta_i \zeta^i$ is a comonic representation of the minimal polynomial of $\mathbf{M}$. Relation (12.15) is achieved by choosing $\mathbf{w}$ in general position with respect to the eigenvectors of $\mathbf{M}$. For example, we could choose

$$\mathbf{M} = \mathsf{diag}\,\{\underbrace{1, 1, \ldots, 1}_{N-\kappa-1},\, 2, \ldots, \kappa\}$$

and $\mathbf{w}$ as a vector of ones.

The first $\kappa + 1$ Krylov vectors $\widehat{\mathbf{r}}_0$, $\widehat{\mathbf{A}}\,\widehat{\mathbf{r}}_0, \ldots, \widehat{\mathbf{A}}^\kappa\,\widehat{\mathbf{r}}_0$ are

$$\begin{bmatrix} 1 \\ 0 \\ \mathbf{w} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}\mathbf{w} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}^2\mathbf{w} \end{bmatrix}, \ldots, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}^\kappa\mathbf{w} \end{bmatrix}.$$

They are linearly independent, hence a basis of $\widehat{\mathcal{K}}_{\kappa+1}$. In view of (12.15) they satisfy

$$\widehat{\mathbf{r}}_0 - \sum_{i=1}^{\kappa} \beta_i \, \widehat{\mathbf{A}}^i \, \widehat{\mathbf{r}}_0 = \mathbf{e}_1 \;\in \mathsf{span}\,\{\mathbf{e}_1\} = \mathcal{N}(\widehat{\mathbf{A}}) \cap \mathcal{Z}^\perp .$$

Consequently, $\mathcal{N}(\widehat{\mathbf{A}}) \cap \widehat{\mathcal{K}}_{\kappa+1} \neq \{\mathbf{o}\}$, whence according to Theorems 2 and 5 deflated GMRES and deflated MINRES (and thus also RMINRES of [62]) break down when attempting to construct $\mathbf{v}_{\kappa+1}$, while, obviously, they do not break down before. To understand this better consider the image of the Krylov basis under the mapping $\widehat{\mathbf{A}}$, which spans $\widehat{\mathbf{A}}\widehat{\mathcal{K}}_{\kappa+1}$:

$$\begin{bmatrix} 0 \\ 0 \\ \mathbf{M}\mathbf{w} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}^2\mathbf{w} \end{bmatrix}, \ldots, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}^\kappa\mathbf{w} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ \mathbf{M}^{\kappa+1}\mathbf{w} \end{bmatrix}.$$

Due to (12.15) these $\kappa + 1$ vectors are linearly dependent, so $\mathsf{dim}\,\widehat{\mathbf{A}}\widehat{\mathcal{K}}_{\kappa+1} = \kappa$ only, which shows that we have Case (i) of Lemma 1, namely a breakdown during step $\kappa + 1$ of the Arnoldi process. Here, $2 \leq \kappa + 1 < N$.

For a breakdown in the first step we could, for example, consider the same type of $\mathbf{A}$ with an arbitrary $\mathbf{M}$ combined with $\mathbf{P} = \mathbf{e}_1\mathbf{e}_1^\mathsf{T}$ and an arbitrary $\mathbf{w}$. Then $\widehat{\mathbf{A}} = \mathbf{O}$, and the method will fail for any initial $\widehat{\mathbf{r}}_0 \neq \mathbf{o}$.

However, as we mentioned in the beginning of Section 3, a breakdown is very unlikely if $\mathcal{Z}$ is chosen such that an approximately invariant subspace is deflated and the deflated eigenvalues are well separated from the not deflated ones. In our example $\mathbf{A}\mathcal{Z} = \mathsf{span}\,\{\mathbf{A}\mathbf{e}_2\} = \mathsf{span}\,\{\mathbf{e}_1\}$, so $\mathcal{Z}$ is not at all approximately invariant.

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