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IDR: A new generation of Krylov subspace methods?☆

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ABSTRACT

The induced dimension reduction (IDR) technique developed by Sonneveld and van Gijzen [1] is a powerful concept resulting in a variety of transpose-free Krylov subspace methods based on short-term recurrences. We present the main differences between and similarities of IDR methods and classical Krylov subspace methods; our tool of trade is the so-called generalized Hessenberg decomposition. The concept of "transfer" of techniques from the setting of (classical) Krylov subspace methods to the IDR based methods is introduced. For simplicity, we only sketch some recent results in the fields of eigenvalue computations and of solution of linear systems.

1. Introduction

IDR [2] by Sonneveld [1] and the more recent generalization IDR(s) [1] by Sonneveld and van Gijzen are transpose-free short-term iterative methods that are linked to variants of Lanczos's process [3,4], namely, to variants with one right-hand and several left-hand starting vectors [5]. There has been an increased interest in IDR based methods [6–16] during the last years, and, at the same time, many have a somewhat skeptical attitude concerning these new developments. The reason for this attitude

☆ Dedicated to the memory of Muharrem Rizvanolli (*08.12.1946–†02.09.2011).

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[1] The article by Wesseling and Sonneveld splits into two clearly separated parts: a part by Wesseling on a multiple grid method and a smaller part by Sonneveld on IDR.

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is simple: The first IDR method that gained popularity was BiCGStab [17,18]. The expectations raised by the introduction of BiCGStab were too high and could not be fulfilled; soon it was realized that BiCGStab was not as stable as anticipated and very sensitive to perturbations. It is not clear *a priori* why IDR(s) should be different. In Section 2 we state the known relation that IDR(s) is a certain two-sided Lanczos with some extra polynomials [13,10], so why should IDR based methods provide something new? It should be obvious by now that an answer to a question raised in the title, namely, if an IDR based method is a *new* Krylov subspace method, alas, is *no*. Yet there are two subtle important differences: the small s attached to the acronym "IDR" with a large impact on the numerical behavior; the derivation of the algorithm without the need for the Lanczos based formalism, thus resulting in a simpler derivation of algorithms and avoiding so called pivot breakdowns. At least in numerical experiments, IDR based methods for moderate values of s are pretty close to Arnoldi based methods and outperform Lanczos based methods. A partial explanation for this observation has been attempted in [14]. The simplified derivation of IDR based methods will eventually result in a *new generation* of methods.

In this contribution we intend to bridge the aforementioned gap between interest and skeptical attitude, to simplify and unify existing theory for IDR based methods, and outline some forthcoming developments.[2] To ease understanding, we organized the paper like a review.

1.1. Motivation

The original IDR method [2] acted as initial nucleus for a rapid development of classical Krylov subspace methods: soon Sonneveld presented CGS [19] and started to work on a reformulation of IDR with van der Vorst, resulting in the famous BiCGStab [17,18]. Original IDR is the forgotten ancestor of a whole branch of new methods, which are frequently termed 'Lanczos-type product methods', 'Hybrid BiCG methods', or 'Krylov product methods'. Below we propose the simpler name *Sonneveld methods* to capture these and those built upon the prototype IDR(s) [1]. The other methods related to original IDR include in succession BiCGStab2 [20], BiCGStab(ℓ) [21], GCGS [22] (in particular CGS2 and shifted CGS), GPBiCG [23], BiCGSafe [24], TFQMR [25], QMRCGStab [26], TFIQMR and TFILanczos [27], and last but not least, ML(k)BiCGStab [28]. All these methods rely on the Lanczos method and can break down for several reasons. The composite step methods by Chan and Szeto [29,30] avoid one type of breakdown, namely, the so-called *pivot breakdown* caused by singularity of the underlying projected tridiagonal matrix of the Lanczos process that is implicitly LDU factorized. Of all the methods mentioned, ML(k)BiCGStab is special in relying on several left-hand starting vectors in the underlying Lanczos process; it is the first transpose-free short-term method of that type.

With IDR(s) [1] a new method of exactly this type has been published. Similarly, despite the fact that Yeung and Chan developed such a method before Sonneveld and van Gijzen, the transition to higher dimensional shadow spaces, as proposed in [1], stirs up a renewed rapid development of new Krylov subspace methods. The reason is simple: the approach of Sonneveld and van Gijzen is based on a *geometric understanding*, namely, the IDR theorem, whereas the approach by Yeung and Chan is a rather technical one that cannot easily be adapted to other flavors of Krylov subspace methods. In this paper we show how to transfer the techniques developed for the original IDR and other Krylov subspace methods to the IDR setting, e.g., to incorporate higher dimensional shadow spaces into well-known approaches. What may appear to be a rather simple technical step offers enhanced convergence properties; Sonneveld methods have the power to bridge the gap between methods based on Lanczos's process and the Arnoldi method [31]. A recent step towards an explanation of this phenomenon is given in [14]; we present numerical experiments to justify this hypothesis, compare with the remarks in [32].

Peter Sonneveld could be titled 'the father of IDR based methods' as he developed the original IDR between 1976 and 1979, came up with CGS, initiated the work on the famous BiCGStab, and finally came up with IDR(s) jointly with Martin B. van Gijzen. To honor Peter Sonneveld, from now on we refer to IDR based methods as *Sonneveld methods*.

[2] We remark that part of the presented results are new, namely, the two extensions of the IDR theorem in Section 2, the sketch of a new IDR variant (our proposed "third approach" in Section 3), and the harmonic Ritz approach for IDR based methods summarized in Eq. (19) and the surrounding text. The pencils for the eigenvalue computations based on IDRBiO and IDRStab are published here for the first time.

1.2. Notation

We use boldface letters to denote matrices and vectors. The identity matrix of size $n \times n$ is denoted by $\mathbf{I}_n$, its columns by $\mathbf{e}_j$, $1 \leqslant j \leqslant n$, and its elements by Kronecker delta δ_{ij}, $1 \leqslant i, j \leqslant n$. A zero matrix of size $n \times k$ is denoted by $\mathbf{O}_{n,k}$, a zero column vector of length k by $\mathbf{o}_k$. We omit indices when they are easily deducible from the context. The matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ is the system matrix of a linear system and/or we are interested in some of its eigenvalues. We remark that we do not impose any further structure on $\mathbf{A}$. The spectrum of $\mathbf{A}$ is denoted by $\sigma(\mathbf{A})$. Column vectors of matrices are denoted by the same letter, e.g., $\mathbf{a}_j \in \mathbb{C}^n$, $1 \leqslant j \leqslant n$, are the column vectors of $\mathbf{A}$. Scalars are denoted by Greek letters, entries of matrices and vectors are denoted by small Roman letters, e.g., a_{ij} is the entry of $\mathbf{A}$ in row i and column j. Spaces are denoted by calligraphic letters like $\mathcal{S}$, $\mathcal{K}_k$, $\mathcal{G}_j$. The letter $\mathcal{S}$ is used in two contexts: as a subspace of codimension s and to denote Sonneveld spaces. The letter $\mathcal{K}$ without index denotes the full Krylov subspace of $\mathbf{A}$ and starting vector $\mathbf{g}_1$. Sonneveld methods are related to a set of basis vectors that live in certain spaces $\mathcal{G}_j$. These are denoted by $\mathbf{g}_k \in \mathbb{C}^n$ and are collected in matrices $\mathbf{G}_k \in \mathbb{C}^{n\times k}$, $1 \leqslant k$. Krylov methods in general, and Sonneveld methods in particular, compute unreduced extended Hessenberg matrices. These are denoted by $\underline{\mathbf{H}}_k \in \mathbb{C}^{(k+1)\times k}$, where the underbar should remind of an additional row vector appended at the bottom of the square upper Hessenberg matrix $\mathbf{H}_k \in \mathbb{C}^{k\times k}$. Sonneveld methods differ from other Krylov subspace methods in constructing additionally upper triangular matrices $\mathbf{U}_k \in \mathbb{C}^{k\times k}$. Variants of $\mathbf{I}_k$ and $\mathbf{U}_k$ exist that carry an additional zero row at the bottom, these are denoted by $\underline{\mathbf{I}}_k$ and $\underline{\mathbf{U}}_k$, respectively, with columns $\underline{\mathbf{e}}_j$ and $\underline{\mathbf{u}}_j$, $1 \leqslant j \leqslant k$. The arising *Sonneveld pencils* $(\mathbf{H}_k, \mathbf{U}_k)$ can be considered as approximations to the pencil $(\mathbf{A}, \mathbf{I}_n)$; the extended pencils $(\underline{\mathbf{H}}_k, \underline{\mathbf{U}}_k)$ are used in methods based on the Minimal Residual (MR) approach. The transpose, the complex conjugate transpose, the (Moore–Penrose) pseudo-inverse, and the inverse are denoted by appending $^{\mathsf{T}}$, $^{\mathsf{H}}$, †, $^{-1}$, respectively. The inclusion and strict inclusion of sets is denoted by $\subseteq$ and $\subset$, respectively. For any $x \in \mathbb{R}$, $\lfloor x \rfloor \in \mathbb{Z}$ denotes the largest integer with $\lfloor x \rfloor \leqslant x$. Similarly, $\lceil x \rceil \in \mathbb{Z}$ denotes the smallest integer with $x \leqslant \lceil x \rceil$. The symbol $\perp$ denotes orthogonality of vectors with respect to the standard Euklidian inner product, $\|\cdot\|$ denotes Euklidian length. The orthogonal complement of a subspace is accordingly denoted by appending $^{\perp}$. The operators dim, codim and ker return the dimension of a vector space, the codimension of a subspace and the kernel of a linear map, respectively. Following [10] we denote names of algorithms in a unified manner, e.g., GMRes in place of GMRES, BiCGStab in place of BiCGstab, and IDRStab as acronym for both methods described in [13,11].

1.3. Outline

We present some basic results in Section 2. We introduce generalized Hessenberg decompositions and Sonneveld pencils in Section 3 and sketch how these can be used to mimic well-known Krylov subspace techniques in the context of Sonneveld methods. In Section 4 we collect the pencils used in the eigenvalue solver counterparts of some recent IDR(s) based linear system solvers and give a few numerical experiments highlighting the differences between them. In Section 5 we focus on the much more advanced situation concerning the solution of linear systems; recent contributions are based on MR approaches in the IDR setting. We conclude in Section 6 and give an outlook.

2. Basics

Sonneveld methods are based on the *IDR spaces* $\mathcal{G}_j$, $0 \leqslant j \leqslant m$, where m is defined later on:

Definition 2.1 (IDR spaces)**.** Let $\mathcal{S}$ be a space of codimension $s \in \mathbb{N}$. Let $\mathcal{G}_0$ be the full Krylov subspace

$$\mathcal{G}_0 := \mathcal{K} = \mathcal{K}_n(\mathbf{A}, \mathbf{g}_1) = \operatorname{span}\{\mathbf{g}_1, \mathbf{A}\mathbf{g}_1, \ldots, \mathbf{A}^{n-1}\mathbf{g}_1\} \subseteq \mathbb{C}^n. \tag{1}$$

Then $\mathcal{G}_j$, $1 \leqslant j \leqslant m$, is defined recursively by

$$\mathcal{G}_j := (\mu_j \mathbf{I} - \mathbf{A})(\mathcal{G}_{j-1} \cap \mathcal{S}), \quad 1 \leqslant j \leqslant m, \tag{2}$$

Table 1
Relations between the various spaces used in this article. All quantities are based on pre-defined $\mathbf{A} \in \mathbb{C}^{n\times n}$, $\mathbf{M}, \widetilde{\mathbf{R}}_0 \in \mathbb{C}^{n\times s}$, $\mathbf{g}_1 \in \mathbb{C}^n$, and the polynomials M_j defined by $M_j(z) := \prod_{i=1}^{j}(\mu_j - z)$ with given $\mu_i \in \mathbb{C}, 1 \leqslant i \leqslant j \leqslant m$.

Symbol	Definition	Name	Comment
$\mathcal{R}$	$\mathcal{R} := \operatorname{span}\{\widetilde{\mathbf{R}}_0\mathbf{e}_1, \ldots, \widetilde{\mathbf{R}}_0\mathbf{e}_s\}$	Shadow space	$\dim(\mathcal{R}) = s$
$\mathcal{S}$	$\mathcal{S} := \mathcal{R}^{\perp}$	Auxiliary IDR space	$\operatorname{codim}(\mathcal{S}) = s$
$\mathcal{K}_k(\mathbf{A}, \mathbf{g}_1)$	$\operatorname{span}\{\mathbf{g}_1, \mathbf{A}\mathbf{g}_1, \ldots, \mathbf{A}^{k-1}\mathbf{g}_1\}$	Krylov subspaces	$k = 0, 1, \ldots$
$\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$	$\left\{\sum_{i=0}^{j-1}(\mathbf{A}^{\mathsf{H}})^i\widetilde{\mathbf{R}}_0\mathbf{c}_i \mid \mathbf{c}_i \in \mathbb{C}^s\right\}$	Krylov subspaces	$j = 0, 1, \ldots$
$\mathcal{S}(P, \mathbf{A}, \mathbf{M})$	$P(\mathbf{A})\left(\mathcal{K}_n(\mathbf{A}, \mathbf{g}_1) \cap \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{M})^{\perp}\right)$	Sonneveld spaces	$j = \deg(P)$
$\mathcal{G}_0$	$\mathcal{K}_n(\mathbf{A}, \mathbf{g}_1)$	Zeroth IDR space	
$\mathcal{G}_j$	$(\mu_j\mathbf{I} - \mathbf{A})(\mathcal{G}_{j-1} \cap \mathcal{S})$	IDR spaces, $j \geqslant 1$	$\mathcal{G}_j = \mathcal{S}(M_j, \mathbf{A}, \widetilde{\mathbf{R}}_0)$

for arbitrary $\mu_j \in \mathbb{C}, 1 \leqslant j \leqslant m$.

If $\mathbf{A}$, $\mathcal{S}$ and all $\mu_j \in \mathbb{C}$ are chosen generically, $m = \lceil n/s \rceil$ and $\mathcal{G}_m = \{\mathbf{o}\}$. For later use we denote the pre-images of the linear mappings $(\mu_j\mathbf{I} - \mathbf{A})$ by $\mathcal{V}_{j-1} := \mathcal{G}_{j-1} \cap \mathcal{S}, 1 \leqslant j \leqslant m$. The IDR spaces are particular cases of *Sonneveld spaces* [13, Definition 2.2, p. 2690]:

Definition 2.2 (Sonneveld spaces)**.** Sonneveld spaces $\mathcal{S}(P, \mathbf{A}, \mathbf{M})$ are subspaces defined by a polynomial P of exact degree j and two matrices $\mathbf{A} \in \mathbb{C}^{n\times n}$ and $\mathbf{M} \in \mathbb{C}^{n\times s}$ as follows,

$$\mathcal{S}(P, \mathbf{A}, \mathbf{M}) := \{P(\mathbf{A})\mathbf{v} \mid \mathbf{v} \in \mathcal{G}_0, \mathbf{v} \perp \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{M})\} = P(\mathbf{A})\left(\mathcal{G}_0 \cap \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{M})^{\perp}\right). \tag{3}$$

Sonneveld spaces are related to left block Krylov subspaces

$$\mathcal{K}_0(\mathbf{A}^{\mathsf{H}}, \mathbf{M}) := \{\mathbf{o}\}, \quad \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{M}) := \left\{\sum_{i=0}^{j-1}(\mathbf{A}^{\mathsf{H}})^i\mathbf{M}\mathbf{c}_i \mid \mathbf{c}_i \in \mathbb{C}^s\right\}, \quad j \geqslant 1, \quad \mathbf{M} \in \mathbb{C}^{n\times s}. \tag{4}$$

Let the columns of $\widetilde{\mathbf{R}}_0 \in \mathbb{C}^{n\times s}$ form a basis of the so-called *shadow space* $\mathcal{S}^{\perp}$ [12, Notation 1]. We state this as $\mathcal{S} = \widetilde{\mathbf{R}}_0^{\perp}$. In [12, Theorem 11, p. 1104, Note 2, p. 1105] it is proven that with $M_j(z) := \prod_{i=1}^{j}(\mu_i - z)$, $j \geqslant 1$, and $M_0(z) := 1$,

$$\mathcal{G}_j = \mathcal{S}(M_j, \mathbf{A}, \widetilde{\mathbf{R}}_0) = \{M_j(\mathbf{A})\mathbf{v} \mid \mathbf{v} \in \mathcal{G}_0, \mathbf{v} \perp \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)\}, \quad 0 \leqslant j \leqslant m. \tag{5}$$

For further reference we collect the notations for all the spaces used frequently throughout this article and the relations between them in Table 1. We remark that we already adapted the notation in the table to our context.

The connection of the IDR spaces to left block Krylov subspaces reveals that IDR methods are based on an underlying Lanczos process, see also [13,10]. Numerical experiments indicate that this Lanczos process is the driving force behind Sonneveld methods. IDR spaces are polynomial images of the orthogonal complement of spaces of increasing dimensions, thus form a sequence of nested spaces of shrinking dimension, hence the name induced dimension reduction (IDR). We fix the index m to be the first index such that no new dimension reduction occurs, i.e., m is the first index such that $\mathcal{G}_{m+1} = \mathcal{G}_m$. Some details are collected in the so-called IDR theorem, which we extend here with respect to the possible additional dimension reduction caused by some of the μ_j, $1 \leqslant j \leqslant m$, being eigenvalues[3]:

Theorem 1 (IDR Theorem, see [1, Theorem 2.1,12, Theorem 7, Corollary 13])**.** *Let the IDR spaces $\mathcal{G}_j$, $0 \leqslant j \leqslant m$, be defined as in Definition 2.1 and characterized by Eq. (5). Suppose that $\mathcal{G}_0$ and $\mathcal{S}$ do not share a nontrivial common invariant subspace*[4] *of $\mathbf{A}$. Then*

[3] This may seem superfluous as the probability that a randomly chosen $\mu \in \mathbb{C}$ is an eigenvalue of a matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ will be zero in the generic case, but the additional dimension reduction plays a vital rôle, e.g., in IDR based methods for finite fields.

[4] This does imply that no eigenvectors of $\mathbf{A}$ that are contained in $\mathcal{G}_0$ are contained in $\mathcal{S}$, i.e., no eigenvector of $\mathbf{A}$ in $\mathcal{G}_0$ is perpendicular to all columns of $\widetilde{\mathbf{R}}_0$.

$$\mathcal{G}_j \subset \mathcal{G}_{j-1}, \quad 1 \leqslant j \leqslant m \leqslant n, \quad \text{and} \quad \mathcal{G}_m = \{\mathbf{o}\}, \tag{6}$$

$$\begin{aligned}\dim(\mathcal{G}_j) = \dim(\mathcal{G}_0) &- \dim(\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)) \\ &- \dim(\ker(M_j(\mathbf{A})) \cap \mathcal{G}_0 \cap \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)^{\perp}) \\ &+ (n - \dim(\mathcal{G}_0 \cup \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)^{\perp})).\end{aligned} \tag{7}$$

In the generic case $\mathbf{A}$ *is non-derogatory,* $\mathbf{g}_1$ *has components in direction of every eigenvector and principal vector, and* $\mathcal{G}_0 = \mathbb{C}^n$*, thus in this case Eq. (7) simplifies to*

$$\dim(\mathcal{G}_j) = n - \dim(\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)) - \dim(\ker(M_j(\mathbf{A})) \cap \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)^{\perp}). \tag{8}$$

In most applications $\mu_i \notin \sigma(\mathbf{A})$*,* $1 \leqslant i \leqslant j$*, i.e.,* $M_j(\mathbf{A})$ *is regular, and thus in this case Eq. (7) simplifies further to*

$$\dim(\mathcal{G}_j) = n - \dim(\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)). \tag{9}$$

Proof. Eq. (6) is contained in [1, Theorem 2.1]. Eq. (9) is [12, Corollary 13]. The steps from Eq. (7) to Eq. (8) and from Eq. (8) to Eq. (9) are trivial. Eq. (7) follows from Eq. (5) utilizing $\dim(\mathbf{B}\mathcal{W}) = \dim(\mathcal{W}) - \dim(\ker(\mathbf{B}) \cap \mathcal{W})$, $\dim(\mathcal{A} \cap \mathcal{B}) = \dim(\mathcal{A}) + \dim(\mathcal{B}) - \dim(\mathcal{A} \cup \mathcal{B})$, and $\dim(\mathcal{W}^{\perp}) = n - \dim(\mathcal{W})$. □

We note that we have two sources for dimension reduction, namely, expansion of the left block Krylov subspace, and roots of the polynomial M_j that are equal to eigenvalues of $\mathbf{A}$. The former indicates that typically we have a reduction by s per step, i.e., unless we have a deflation in the left block Krylov subspace. The latter usually is negligible but may be of importance in linear system solvers for finite fields and singular matrices. To understand some of the subtleties attached to singular matrices, we present an academic example:

Example 2.1 (Higher dimension reduction)**.** Let

$$\mathbf{A} := \begin{pmatrix} 0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{pmatrix}, \qquad \begin{aligned} \mathbf{g}_1 &:= \mathbf{e}_{n-k+1}, && 1 \leqslant k \leqslant n, \\ \widetilde{\mathbf{R}}_0 &:= \begin{pmatrix} \mathbf{e}_l & \mathbf{e}_{l+p} \end{pmatrix}, && 1 \leqslant l < l+p \leqslant n. \end{aligned}$$

Then $\mathcal{G}_0 = \operatorname{span}\{\mathbf{e}_{n-k+1}, \ldots, \mathbf{e}_n\}$, i.e., $\dim(\mathcal{G}_0) = k$. Observe that the assumptions of Theorem 1 are violated when $l + p < n$, as the eigenvector $\mathbf{e}_n$ satisfies $\mathbf{e}_n \in \mathcal{G}_0 \cap \mathcal{S}$. We set all $\mu_i = 0$, $1 \leqslant i \leqslant j$. The intersection with $\mathcal{S} = \widetilde{\mathbf{R}}_0^{\perp}$ removes the standard unit vectors with indices l and $l+p$, the multiplication with the shift-down operator $\mathbf{A}$ increases the indices by one and maps $\mathbf{e}_n$ to zero:

$$\begin{aligned}\mathcal{G}_1 &= \mathbf{A}(\mathcal{G}_0 \cap \widetilde{\mathbf{R}}_0^{\perp}) = \mathbf{A} \operatorname{span}\{\mathbf{e}_{n-k+1}, \ldots, \check{\mathbf{e}}_l, \ldots, \check{\mathbf{e}}_{l+p}, \ldots, \mathbf{e}_n\} \\ &= \operatorname{span}\{\mathbf{e}_{n-k+2}, \ldots, \check{\mathbf{e}}_{l+1}, \ldots, \check{\mathbf{e}}_{l+p+1}, \ldots, \mathbf{e}_n\},\end{aligned}$$

here, e.g., $\check{\mathbf{e}}_l$ indicates that the standard unit vector with index l is missing. Similarly,

$$\begin{aligned}\mathcal{G}_2 &= \operatorname{span}\{\mathbf{e}_{n-k+3}, \ldots, \check{\mathbf{e}}_{l+1}, \check{\mathbf{e}}_{l+2}, \ldots, \check{\mathbf{e}}_{l+p+1}, \check{\mathbf{e}}_{l+p+2}, \ldots, \mathbf{e}_n\}, \\ \mathcal{G}_3 &= \operatorname{span}\{\mathbf{e}_{n-k+4}, \ldots, \check{\mathbf{e}}_{l+1}, \check{\mathbf{e}}_{l+2}, \check{\mathbf{e}}_{l+3}, \ldots, \check{\mathbf{e}}_{l+p+1}, \check{\mathbf{e}}_{l+p+2}, \check{\mathbf{e}}_{l+p+3}, \ldots, \mathbf{e}_n\},\end{aligned}$$

and so forth. If $n - k + 3 < l, p > 2$, and $l + p + 3 \leqslant n$, the dimensions of the IDR spaces are given by

$$\dim(\mathcal{G}_0) = k, \quad \dim(\mathcal{G}_1) = k - 3, \quad \dim(\mathcal{G}_2) = k - 6, \quad \dim(\mathcal{G}_3) = k - 9.$$

In general, we observe a dimension reduction of $3 = s + 1$ for $\mathcal{G}_j$ as long as $n - k + j < l, j \leqslant p$, and $l + p + j \leqslant n$. When $n - k + j \geqslant l$ or $j > p$, we have a deflation in the left block Krylov subspace. Depending on $k, l, p \in \mathbb{N}$ we achieve different behavior, but in general we start with a reduction of $3 = s + 1$, this drops to $2 = s$, then to $1 = s - 1$ until we end up with $\mathcal{G}_m = \{\mathbf{o}\}$.

We sketch a simple theoretical generalization of the IDR theorem and provide an alternate description of the resulting spaces, similar to [12, Corollary 13] based on the original proof of the IDR theorem by Sonneveld given in [10].

Theorem 2 (Perturbed IDR Theorem)**.** *Let $\mathcal{G}_0$ be the full Krylov subspace $\mathcal{K}_n(\mathbf{A}, \mathbf{g}_1)$. Define*

$$\mathcal{G}_j := (\mu_j \mathbf{I} - \mathbf{A})(\mathcal{G}_{j-1} \cap \mathcal{S}_j), \quad \operatorname{codim}(\mathcal{S}_j) = s, \tag{10}$$

for $\mu_j \in \mathbb{C}$ and possibly different subspaces $\mathcal{S}_j$, $1 \leqslant j \leqslant m$.
Then

$$\mathcal{G}_j = M_j(\mathbf{A})\mathcal{G}_0 \cap \left(\bigcap_{i=1}^{j} (\mu_j \mathbf{I} - \mathbf{A}) \cdots (\mu_i \mathbf{I} - \mathbf{A})\mathcal{S}_i \right). \tag{11}$$

Suppose that no μ_i, $1 \leqslant i \leqslant j$ is equal to an eigenvalue of $\mathbf{A}$. Let matrices $\widetilde{\mathbf{R}}_0^{(j)}$, $1 \leqslant j \leqslant m$, be given with $\mathcal{S}_j = (\widetilde{\mathbf{R}}_0^{(j)})^{\perp}$. Denote $\mathcal{R}_j := \operatorname{span}\{\widetilde{\mathbf{R}}_0^{(j)}\} = \mathcal{S}_j^{\perp}$. Then

$$\mathcal{G}_j = \mathcal{G}_0 \cap \left(\bigcap_{i=1}^{j} (\mu_j \mathbf{I} - \mathbf{A}) \cdots (\mu_i \mathbf{I} - \mathbf{A})\mathcal{S}_i \right) = \mathcal{G}_0 \cap \left(\bigcap_{i=0}^{j-1} M_i(\mathbf{A})^{-1} M_j(\mathbf{A})\mathcal{S}_{j-i} \right) \tag{12a}$$

$$= \mathcal{G}_0 \cap \left(\bigcup_{i=0}^{j-1} M_j(\mathbf{A})^{-\mathsf{H}} M_i(\mathbf{A})^{\mathsf{H}} \mathcal{R}_{j-i} \right)^{\perp} = \mathcal{G}_0 \cap M_j(\mathbf{A}) \left(\bigcup_{i=0}^{j-1} M_i(\mathbf{A})^{\mathsf{H}} \mathcal{R}_{j-i} \right)^{\perp} \tag{12b}$$

Proof. Eq. (11) is trivial and follows from the fact that $\mathbf{B}(\mathcal{A} \cap \mathcal{B}) = \mathbf{B}\mathcal{A} \cap \mathbf{B}\mathcal{B}$ for matrices $\mathbf{B}$ and subspaces $\mathcal{A}$ and $\mathcal{B}$. Since $\mathcal{G}_0$ is an invariant subspace of $\mathbf{A}$, $M_j(\mathbf{A})\mathcal{G}_0 \subseteq \mathcal{G}_0$. We have equality, as $M_j(\mathbf{A})$ is regular by assumption. All inverses in the second equality in Eq. (12a) are well-defined as all $\mu_i \notin \sigma(\mathbf{A})$. The first equality in Eq. (12b) is based on $\mathcal{A}^{\perp} \cap \mathcal{B}^{\perp} = (\mathcal{A} \cup \mathcal{B})^{\perp}$; both equalities in Eq. (12b) use $\mathbf{B}\mathcal{W}^{\perp} = (\mathbf{B}^{-\mathsf{H}}\mathcal{W})^{\perp}$ for any regular matrix $\mathbf{B}$. □

The *generalized Sonneveld spaces* defined as

$$\mathcal{S}(M_1, \ldots, M_j, \mathbf{A}, \widetilde{\mathbf{R}}_0^{(1)}, \ldots, \widetilde{\mathbf{R}}_0^{(j)}) := M_j(\mathbf{A}) \left(\bigcup_{i=0}^{j-1} M_i(\mathbf{A})^{\mathsf{H}} \mathcal{R}_{j-i} \right)^{\perp} \tag{13}$$

are again polynomial images of the orthogonal complement of, in the generic case, spaces of growing dimensions, thus, polynomial images of spaces of shrinking dimensions.

This *perturbed IDR theorem* and the generalized Sonneveld spaces are a generalization of the IDR theorem and the Sonneveld spaces: when all $\widetilde{\mathbf{R}}_0^{(i)}$, $1 \leqslant i \leqslant j$, are equal, we recover the IDR theorem and the Sonneveld spaces, as the polynomials form a basis of the polynomials of degree less j. The perturbed IDR theorem is applicable when all $\widetilde{\mathbf{R}}_0^{(i)}$, $1 \leqslant i \leqslant j$, are perturbations of a single $\widetilde{\mathbf{R}}_0$, e.g., because of finite precision computations, hence the name.

The IDR theorem forms the basis for vector recurrences with finite termination property where only as many vectors as needed at most are computed. The vectors constructed and the recurrence coefficients can be captured in the form of a matrix equation, a so-called *generalized Hessenberg decomposition* [10]. This is described in the next section.

3. Generalized Hessenberg decompositions

The IDR theorem is a theorem about nested spaces. To translate this theorem into an algorithm, we need a recurrence of sets of vectors. Typically, the full Krylov subspace $\mathcal{G}_0$ will be of dimension n, which is large, and it will be prohibitive to store a full basis. Even though the dimension of every next $\mathcal{G}_j, j \geqslant 1$, will be smaller, the reduction will not be substantial; usually the algorithm will be terminated before we can afford to store a full basis of any implicitly described $\mathcal{G}_j, j \geqslant 1$. It turns out to be possible to compute vectors in IDR spaces with higher index j without the need for a basis of any $\mathcal{G}_0, \mathcal{G}_1, \ldots, \mathcal{G}_{j-1}$. The crucial point is the computation of a vector that lies in the intersection with $\mathcal{S}$, as polynomial images of vectors can be computed without the need for other vectors in that space.

In the generic case we need at least $s+1$ vectors in $\mathcal{G}_{j-1}, j \geqslant 1$, to compute a non-trivial vector in the intersection $\mathcal{V}_{j-1} = \mathcal{G}_{j-1} \cap \mathcal{S}$. In $\mathcal{G}_0$, mostly any basis $\mathbf{g}_1, \ldots, \mathbf{g}_s$ of $\mathcal{K}_s = \mathcal{K}_s(\mathbf{A}, \mathbf{g}_1)$ and one vector from $\mathcal{K}_{s+1} \setminus \mathcal{K}_s$, e.g., $\mathbf{A}\mathbf{g}_s$, is used to compute $\mathbf{g}_{s+1} \in \mathcal{V}_0 \subset \mathcal{G}_0$. For stability reasons we advocate to use Arnoldi's method resulting in an *Arnoldi decomposition* $\mathbf{A}\mathbf{G}_{s-1} = \mathbf{G}_s \underline{\mathbf{H}}_{s-1}$ with orthonormal $\mathbf{G}_s = (\mathbf{g}_1, \ldots, \mathbf{g}_s) \in \mathbb{C}^{n \times s}$ and extended upper Hessenberg $\underline{\mathbf{H}}_{s-1} \in \mathbb{C}^{s \times (s-1)}$. To determine a first vector in the intersection $\mathcal{V}_0 = \mathcal{G}_0 \cap \mathcal{S}$, we need one additional vector $\mathbf{g}_{s+1} \in \mathcal{G}_0$.

For this vector $\mathbf{g}_{s+1}$ there are basically three simple choices: use $\mathbf{A}\mathbf{g}_s$, use Arnoldi also for $\mathbf{g}_{s+1}$ or, where we assume that $\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_s$ is regular, normalize $\mathbf{A}\mathbf{g}_s - \mathbf{G}_s\mathbf{c}$, where $\mathbf{c} \in \mathbb{C}^s$ solves $\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_s \mathbf{c} = \widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{A}\mathbf{g}_s$. This vector has to be computed in any case. The first choice is natural, as multiplication of the last basis vector $\mathbf{g}_s$ by $\mathbf{A}$ is the traditional way to expand a Krylov subspace. In the second choice, based on Arnoldi's method, we trade additional work in for the advantage to be equipped with an orthonormal basis of $\mathcal{G}_0 \setminus \mathcal{G}_1$. A vector in the intersection, which is needed in the algorithm, is given by the third choice $\mathbf{A}\mathbf{g}_s - \mathbf{G}_s\mathbf{c}$. The vector $\mathbf{A}\mathbf{g}_s$ has to be computed in any case. The reason to consider the other choices is that in later steps we need a basis of $\mathcal{G}_0 \setminus \mathcal{G}_1$ and the behavior of algorithm depends, among others, on the properties of that basis.

Once we have picked any of the three choices, we need s additional vectors to compute the first vector in the next intersection. We treat three different approaches to compute additional vectors in Sonneveld methods. To simplify the exposition we assume that no deflation occurs in the left block Krylov subspaces and that $\mu_j \notin \sigma(\mathbf{A}), j \geqslant 1$.

The computation of new vectors in $\mathcal{G}_j$ is based on $\mathcal{G}_j \subset \mathcal{G}_{j-1}$, i.e., Eq. (6): given $s+1$ vectors in $\mathcal{G}_{j-1}$, we can compute one vector in $\mathcal{V}_{j-1}$, which is essentially unique, choose μ_j and map it to a vector in $\mathcal{G}_j$ *and also in* $\mathcal{G}_{j-1}$. Suppose we have $s+k$ linearly independent vectors in $\mathcal{G}_{j-1}$, then typically the intersection $\mathcal{V}_{j-1}$ with $\mathcal{S}$ has dimension k and we can compute k vectors in $\mathcal{G}_j$. Thus, to obtain $s+1$ vectors in $\mathcal{G}_j$, we need $2s+1$ vectors in $\mathcal{G}_{j-1}$. There are different ways to compute vectors in the intersection $\mathcal{V}_{j-1}$.

The approaches in [1,33,11,32] use only the last $s+1$ $\mathbf{g}$-vectors, thus implementing the shortest recurrence possible. A prototype implementation of this scheme is given by

$$\begin{aligned} &\mathbf{v}_k := \mathbf{g}_k - \mathbf{G}_{k-s:k-1}\mathbf{c}_k \in \mathcal{V}_{j-1}, \quad \text{where} \quad \mathbf{c}_k := (\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{k-s:k-1})^{-1} (\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{g}_k), \\ &\mathbf{g}_{k+1} := (\mu_j \mathbf{I} - \mathbf{A})\mathbf{v}_k \in \mathcal{G}_j \subset \mathcal{G}_{j-1}. \end{aligned} \tag{14}$$

Additionally, a basis transformation of the vectors we already have computed in $\mathcal{G}_j$ can be utilized. The disadvantage of this scheme is that the projection matrix $\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{k-s:k-1}$ has to be updated in every step, the part of the work for the projection per step is $O(s^3)$. In [33] the projection matrices are nested upper triangular; the complexity drops to $O(s^2)$ per step, at the cost of additional vector updates with long vectors.

In [13] a fixed set of s vectors is used, the projection matrix remains the same and needs to be factored only once every $s+1$ steps. In contrast to the first group of approaches, this is a $2s+1$ term recurrence. As a basis transformation the resulting $\mathbf{g}$-vectors in $\mathcal{G}_j$ are orthonormalized.

In both these groups of approaches the projection matrices may be ill-conditioned leading to large projection coefficients $\mathbf{c} \in \mathbb{C}^s$. We remark that the first vector in $\mathcal{G}_j$ is computed using the same projection in *every* possible approach.

We propose a third approach: we use all available vectors in $\mathcal{G}_{j-1}$ to compute a minimum norm solution in the projection step, i.e., for $0 \leqslant i \leqslant s$ and for $j \geqslant 1$,

$$\begin{aligned} \mathbf{v}_{j(s+1)+i} &:= \mathbf{g}_{j(s+1)+i} - \mathbf{G}_{(j-1)(s+1)+1:j(s+1)+i-1}\mathbf{c}_i \in \mathcal{V}_{j-1}, \\ &\text{where} \quad \mathbf{c}_i := (\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{(j-1)(s+1)+1:j(s+1)+i-1})^{\dagger}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{g}_{j(s+1)+i}), \\ \mathbf{g}_{j(s+1)+i+1} &:= (\mu_j\mathbf{I} - \mathbf{A})\mathbf{v}_{j(s+1)+i} \in \mathcal{G}_j \subset \mathcal{G}_{j-1}. \end{aligned} \tag{15}$$

The resulting $\mathbf{g}$-vectors in $\mathcal{G}_j$ are then orthonormalized. Numerical experiments indicate that this third approach is slightly more robust than the other two. The additional cost for computing the minimum norm solution is of order $O(s^3)$; this is negligible for small s.

In Sonneveld methods we capture the computation of the basis vectors $\mathbf{g}_\ell$, $1 \leqslant \ell \leqslant k+1$, in matrix form, a so-called *generalized Hessenberg decomposition* [10]:

$$\mathbf{A}\mathbf{V}_k = \mathbf{A}\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k. \tag{16}$$

Here, $\mathbf{G}_{k+1} = (\mathbf{G}_k, \mathbf{g}_{k+1}) = (\mathbf{g}_1, \ldots, \mathbf{g}_{k+1}) \in \mathbb{C}^{n\times(k+1)}$ accounts for the basis vectors,[5] $\mathbf{U}_k \in \mathbb{C}^{k\times k}$ is upper triangular and captures the projection coefficients $\mathbf{c}_\ell$, and $\underline{\mathbf{H}}_k$ is extended unreduced (upper) Hessenberg and defined in terms of the basis transformations in $\mathcal{G}_j$ and the projection coefficients $\mathbf{c}_\ell$ weighted by μ_j. The matrix $\mathbf{V}_k$ contains the vectors we computed in some $\mathcal{V}_{j-1}$ in its columns. Both $\mathbf{U}_k$ and $\underline{\mathbf{H}}_k$ are banded, the exact structure depends on the IDR variant used. In contrast, essentials of classical Krylov subspace methods [34,3,4,31,35] for $\mathbf{A} \in \mathbb{C}^{n\times n}$ can be described by a *Hessenberg decomposition*, which is the special case $\mathbf{U}_k = \mathbf{I}_k$ and thus $\mathbf{V}_k = \mathbf{G}_k$ of the generalized Hessenberg decomposition (16). In [32] we need another generalization of Eq. (16) obtained when the middle term is missing, e.g., when an upper triangular $\mathbf{U}_k$ with $\mathbf{V}_k = \mathbf{G}_k\mathbf{U}_k$ not necessarily exists. This special case occurs in flexible IDR variants and is referred to as *generalized Hessenberg relation*.

IDR is a Petrov–Galërkin approach, see [9]. The left subspace $\mathcal{L}_{j(s+1)+i}$, $0 \leqslant i \leqslant s$, is given by $\mathcal{L}_{j(s+1)+i} = M_j(\mathbf{A})^{-\mathsf{H}}\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0)$, $1 \leqslant j \leqslant m$, [9, Eq. (3.3)], the right subspace by $\mathcal{K}_{k+1}$, $k = j(s+1)+i$. If $\operatorname{rank}(\mathbf{G}_{k+1}) = k+1$, the rectangular extended Sonneveld pencil $(\underline{\mathbf{H}}_k, \underline{\mathbf{U}}_k)$ can be interpreted as rectangular projection of the pencil $(\mathbf{A}, \mathbf{I}_n)$:

$$\mathbf{G}_{k+1}^{\dagger}(\mathbf{A}, \mathbf{I}_n)\mathbf{G}_{k+1}\underline{\mathbf{U}}_k = \mathbf{G}_{k+1}^{\dagger}(\mathbf{A}\mathbf{G}_k\mathbf{U}_k, \mathbf{G}_{k+1}\underline{\mathbf{U}}_k) = \mathbf{G}_{k+1}^{\dagger}(\mathbf{G}_{k+1}\underline{\mathbf{H}}_k, \mathbf{G}_{k+1}\underline{\mathbf{U}}_k) = (\underline{\mathbf{H}}_k, \underline{\mathbf{U}}_k). \tag{17}$$

Here, $\underline{\mathbf{U}}_k \in \mathbb{C}^{(k+1)\times k}$ denotes $\mathbf{U}_k$ with a zero row appended at the bottom. In classical Krylov methods we only have to consider $\underline{\mathbf{H}}_k$ and its leading square part $\mathbf{H}_k$. It turns out that we can transfer most techniques known for classical Krylov subspace methods to Sonneveld methods, we only have to insert the upper triangular $\mathbf{U}_k$ at the correct places. We briefly sketch the resulting Ritz, harmonic Ritz, Orthogonal Residual (OR), and Minimal Residual (MR) approaches.[6] Some further extensions like flexible and multi-shift variants are described in [32]. All these approaches collapse to their well-known counterparts when $\mathbf{U}_k = \mathbf{I}_k$.

The Ritz approach is based on the Sonneveld pencil $(\mathbf{H}_k, \mathbf{U}_k)$, the leading square part of the extended Sonneveld pencil $(\underline{\mathbf{H}}_k, \underline{\mathbf{U}}_k)$ [10]. Let $\mathbf{s}_i$ and θ_i be defined by

$$\mathbf{H}_k\mathbf{s}_i = \theta_i\mathbf{U}_k\mathbf{s}_i, \quad \mathbf{y}_i := \mathbf{V}_k\mathbf{s}_i = \mathbf{G}_k\mathbf{U}_k\mathbf{s}_i. \tag{18}$$

Some of the Sonneveld Ritz values θ_i coincide with the values μ_j. The other Sonneveld Ritz pairs $(\theta_i, \mathbf{y}_i)$ can be used as approximations to eigenpairs of $\mathbf{A}$.

In the Sonneveld harmonic Ritz approach with shift $\tau \in \mathbb{C}$ we proceed as follows. Let $\underline{\mathbf{s}}_i$ and $\underline{\theta}_i$ be defined by

$$\mathbf{I}_k\underline{\mathbf{s}}_i = (\underline{\theta}_i - \tau)(\underline{\mathbf{H}}_k - \tau\underline{\mathbf{U}}_k)^{\dagger}\underline{\mathbf{U}}_k\underline{\mathbf{s}}_i, \quad \underline{\mathbf{y}}_i := \mathbf{V}_k\underline{\mathbf{s}}_i = \mathbf{G}_k\mathbf{U}_k\underline{\mathbf{s}}_i. \tag{19}$$

[5] Provided no breakdown occurs, $\mathcal{K}_{k+1}(\mathbf{A}, \mathbf{g}_1) = \operatorname{span}\{\mathbf{g}_1, \ldots, \mathbf{g}_{k+1}\}$.

[6] The approaches labeled "OR" and "MR" are paradigms to construct approximations to the solution of a linear system. We use these terms in a fairly broad sense, see their formal definition on page 1048, Eqs. (20) and (23).

Some of the resulting Sonneveld harmonic Ritz pairs $(\theta_i, \underline{\mathbf{y}}_i)$ with shift τ are approximations to some eigenpairs of $\mathbf{A}$. In an implementation a pencil similar to $(\mathbf{I}_k, (\underline{\mathbf{H}}_k - \tau\underline{\mathbf{U}}_k)^\dagger\underline{\mathbf{U}}_k)$ is used; no pseudo-inverse is computed. Using the extended Sonneveld pencil $(\underline{\mathbf{H}}_k, \underline{\mathbf{U}}_k)$ 'as is' implies that the roots μ_ℓ, $1 \leqslant \ell \leqslant j$, of the polynomials M_j are mixed with genuine eigenvalue approximations.

In both approaches for the computation of eigenvalues a purified and/or a deflated pencil can be used. Purification and deflation have been introduced in [10]: purification moves the known eigenvalues μ_j of the Sonneveld pencil to infinite eigenvalues; deflation removes these infinite eigenvalues and constructs a smaller pencil. In the report [10] the non-trivial computation of Ritz vectors is sketched for purified/deflated IDR pencils, an extension to harmonic Ritz vectors still has to be done.

Most common Krylov subspace methods for solving linear systems can be classified into Orthogonal Residual (OR) approaches and Minimal Residual (MR) approaches. We suppose that $\mathbf{g}_1 = \mathbf{r}_0/\|\mathbf{r}_0\|$, where $\mathbf{Ax} = \mathbf{r}_0$ has to be solved. Both approaches select a coefficient vector $\mathbf{z}_k \in \mathbb{C}^k$ such that $\mathbf{x}_k = \mathbf{V}_k\mathbf{z}_k$ has certain properties. The IDR variants in [1,33,11,13] are of type OR, the IDR variants in [15,32] are of type MR.

The OR approach is based on the small linear Hessenberg system $\mathbf{H}_k\mathbf{z}_k = \mathbf{e}_1\|\mathbf{r}_0\|$. It is not always possible to solve this system, i.e., to use the OR approach. If $\mathbf{H}_k$ is regular, then

$$\mathbf{z}_k := \mathbf{H}_k^{-1}\mathbf{e}_1\|\mathbf{r}_0\|, \quad \mathbf{x}_k := \mathbf{V}_k\mathbf{z}_k = \mathbf{G}_k\mathbf{U}_k\mathbf{z}_k. \tag{20}$$

Suppose that $\mathbf{G}_{k+1}$ has full column rank. Define $\widehat{\mathbf{G}}_k^{\mathsf{H}} := \underline{\mathbf{I}}_k^{\mathsf{T}}\mathbf{G}_{k+1}^\dagger$, i.e., $\widehat{\mathbf{G}}_k^{\mathsf{H}}\mathbf{G}_k = \mathbf{I}_k$ and $\widehat{\mathbf{G}}_k^{\mathsf{H}}\mathbf{g}_{k+1} = \mathbf{o}_k$. The kth residual is orthogonal to the columns of this $\widehat{\mathbf{G}}_k$, which justifies the name OR:

$$\widehat{\mathbf{G}}_k^{\mathsf{H}}\mathbf{r}_k = \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{r}_0 - \mathbf{A}\mathbf{x}_k) = \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{G}_k\mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{A}\mathbf{V}_k\mathbf{z}_k) = \mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{H}_k\mathbf{z}_k = \mathbf{o}_k. \tag{21}$$

The norm of the kth OR residual can be estimated using $\|\mathbf{g}_{k+1}\|$ and $|h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}\mathbf{z}_k|$:

$$\mathbf{r}_k = \mathbf{r}_0 - \mathbf{A}\mathbf{x}_k = \mathbf{G}_k(\mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{H}_k\mathbf{z}_k) - \mathbf{g}_{k+1}h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}\mathbf{z}_k = -\mathbf{g}_{k+1}h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}\mathbf{z}_k. \tag{22}$$

We remark that the OR residuals are always parallel to the basis vectors. Especially, in case of an orthonormal $\mathbf{G}_{k+1}$, $\widehat{\mathbf{G}}_k = \mathbf{G}_k$ and thus $\mathbf{r}_k \perp \mathbf{r}_j$, $0 \leqslant j < k$.

The MR approach is based on the small least-squares problem $\|\underline{\mathbf{H}}_k\underline{\mathbf{z}}_k - \underline{\mathbf{e}}_1\|\mathbf{r}_0\|\| = \min$. This problem is always uniquely solvable, as $\underline{\mathbf{H}}_k$ is unreduced Hessenberg and thus has rank k. We set

$$\underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^\dagger\underline{\mathbf{e}}_1\|\mathbf{r}_0\|, \quad \underline{\mathbf{x}}_k := \mathbf{V}_k\underline{\mathbf{z}}_k = \mathbf{G}_k\mathbf{U}_k\underline{\mathbf{z}}_k. \tag{23}$$

Define $\rho_k := \|\underline{\mathbf{H}}_k\underline{\mathbf{z}}_k - \underline{\mathbf{e}}_1\|\mathbf{r}_0\|\|$. Then the norm of the kth MR residual $\underline{\mathbf{r}}_k$ can be estimated by

$$\|\underline{\mathbf{r}}_k\| = \|\mathbf{r}_0 - \mathbf{A}\underline{\mathbf{x}}_k\| = \|\mathbf{G}_{k+1}(\underline{\mathbf{e}}_1\|\mathbf{r}_0\| - \underline{\mathbf{H}}_k\underline{\mathbf{z}}_k)\| \leqslant \|\mathbf{G}_{k+1}\| \cdot \rho_k. \tag{24}$$

Suppose that $\|\mathbf{g}_j\| = 1$, $1 \leqslant j \leqslant k+1$. Then $\|\mathbf{G}_{k+1}\| \leqslant \sqrt{k+1}$. More refined bounds are possible in case of additional structure, see Lemma 4 in Section 5.2, page 1058. If $\mathbf{G}_{k+1}$ is orthonormal, $\|\underline{\mathbf{r}}_k\| = \rho_k$ and we have a genuine residual minimization, which justifies the name MR.

4. Eigenvalue computations

The computation of eigenvalues based on IDR has been first considered in [10] for the prototype IDR(s) [1]. In [36] these results were extended to the IDR(s) variant described in [33]; in [37] the extension to the generalization IDRSTAB [13] of IDR that allows for stabilizing polynomials of higher degree was considered. For the reader's convenience we gather the results obtained in [10,36,37] in this section and refer to [10] for the proofs. The knowledge about the properties of the pencils for eigenvalue computations obtained in [10,36,37] deepen our understanding and are a first step towards a "genuine" eigenvalue solver based on IDR. The eigenvalue computations contained in [10,36,37] use IDR methods that have been developed for *linear systems* without any changes to better fit them to the

different task of *eigenvalue computations*. We are currently investigating the influences of the choice of parameters in IDR based methods designed *explicitly* for eigenvalue computations.

4.1. The prototype IDR (s) [1]

In the terminology of [10] the prototype IDR(s) is of type OREs and denoted by IDR(s)OREs. OREs methods directly compute residuals but are potentially highly unstable. The recurrences of IDR(s)OREs [1, bottom of page 1039] have been reformulated in [10, Eqs. (4.4)+(4.5)],

$$\mathbf{v}_{k-1} = \mathbf{r}_{k-1} - \sum_{\ell=0}^{s-1} (\mathbf{r}_{k-s+\ell} - \mathbf{r}_{k-s+\ell-1})\gamma_{\ell+1}^{(k)} \in \mathcal{V}_{j-1}, \quad \mathbf{r}_k = (\mathbf{I}_n - \omega_j \mathbf{A})\mathbf{v}_{k-1} \in \mathcal{G}_j. \tag{25}$$

Here the parameters γ are chosen such that $\mathbf{v}_{k-1} \in \mathcal{S}$. Sorting terms results in the kth column of a generalized Hessenberg decomposition. Collecting all columns we obtain the IDR(s)OREs generalized Hessenberg decomposition

$$\mathbf{A}\mathbf{R}_k \mathbf{U}_k^{\text{IDROREs}} = \mathbf{R}_{k+1} \underline{\mathbf{H}}_k^{\text{IDROREs}}, \quad \mathbf{R}_{k+1} = \begin{pmatrix} \mathbf{R}_k & \mathbf{r}_k \end{pmatrix} = \begin{pmatrix} \mathbf{r}_0 & \cdots & \mathbf{r}_{k-1} & \mathbf{r}_k \end{pmatrix}, \tag{26}$$

with the extended IDR(s)OREs Sonneveld pencil [10, Definition 4.4, p. 14] ($\underline{\mathbf{H}}_k^{\text{IDROREs}}$, $\mathbf{U}_k^{\text{IDROREs}}$)

$$\underline{\mathbf{H}}_k^{\text{IDROREs}} = \underline{\mathbf{Y}}_k^{\circ}, \quad \mathbf{U}_k^{\text{IDROREs}} = \mathbf{Y}_k \mathbf{D}_{\omega}^{(k)}, \tag{27}$$

where the upper triangular banded $\mathbf{Y}_k \in \mathbb{C}^{k\times k}$ and the extended unreduced upper Hessenberg banded $\underline{\mathbf{Y}}_k^{\circ} \in \mathbb{C}^{(k+1)\times k}$ are defined by the starting Krylov subspace method used to compute a basis for $\mathcal{K}_{s+1}$ and then columnwise in terms of the intersection parameters γ by

$$\mathbf{Y}_k \mathbf{e}_i := \begin{pmatrix} \mathbf{o}_{i-(s+1)} \\ \gamma_1^{(i)} \\ \gamma_2^{(i)} - \gamma_1^{(i)} \\ \vdots \\ \gamma_s^{(i)} - \gamma_{s-1}^{(i)} \\ 1 - \gamma_s^{(i)} \\ \mathbf{o}_{k-i} \end{pmatrix}, \quad \underline{\mathbf{Y}}_k^{\circ} \mathbf{e}_i := \begin{pmatrix} \mathbf{o}_{i-(s+1)} \\ \gamma_1^{(i)} \\ \gamma_2^{(i)} - \gamma_1^{(i)} \\ \vdots \\ \gamma_s^{(i)} - \gamma_{s-1}^{(i)} \\ 1 - \gamma_s^{(i)} \\ -1 \\ \mathbf{o}_{k-i} \end{pmatrix}, \quad s < i \leqslant k. \tag{28}$$

The parameters ω enter the scene only in the diagonal matrix $\mathbf{D}_{\omega}^{(k)} \in \mathbb{C}^{k\times k}$ defined by $\mathbf{e}_i^{\mathsf{T}} \mathbf{D}_{\omega}^{(k)} \mathbf{e}_i = \omega_j$, $j = \lfloor i/(s+1) \rfloor$, c.f. [10, Theorem 4.1]. For every completed ω_j-block this Sonneveld pencil by structure has an eigenvalue $1/\omega_j$, c.f. [10]. Setting all elements in certain upper triangular parts of $\mathbf{Y}_k$ to zero results in the purified IDR(s)OREs pencil [10, Theorem 4.8] that has the same eigenvalues as the IDR(s)OREs Sonneveld pencil, but the roots $1/\omega_j$ of the Omega polynomials have been replaced by infinite eigenvalues. Taking a Schur complement gives a deflated IDR(s)OREs pencil of smaller size that has only genuine eigenvalue approximations. These can be identified with those of a Lanczos(s, 1) process; it is easy to construct the coefficients of this Lanczos(s, 1) process from the deflated IDR(s)OREs pencil. For details we refer to the report [10]; we explicitly mention that the computation of Ritz values using the Sonneveld pencil is often badly conditioned and we propose to use either a purified or deflated pencil. To be more precise, the condition numbers of those Ritz values that are approximations to eigenvalues of $\mathbf{A}$ are much larger than the condition numbers of the eigenvalues of $\mathbf{A}$ that they approx-

imate. In contrast, the Ritz values close to the roots $1/\omega_j$ are usually better conditioned. This sensitive behavior is reflected in the unstable behavior of the prototype IDR(s), especially for large values of s, as a linear system solver.

4.2. *"Elegant"* IDR(s) *[33]*

In the generic case the first vector in a new space $\mathcal{G}_j$ is uniquely defined up to scaling. Once we have computed some vectors in a new space $\mathcal{G}_j$, we can chose any linear combinations as new basis vectors that have better properties. This was first used in [33], e.g., to generate basis vectors and residuals $\mathbf{g}_{j(s+1)+i+1}, \mathbf{r}_{j(s+1)+i+1} \in \mathcal{G}_j$, $0 \leqslant i \leqslant s$, that are orthogonal to the first $i-1$ and i columns $\widetilde{\mathbf{r}}_\ell^{(0)}$ of $\widetilde{\mathbf{R}}_0$, [33, p. 5:6, Eqs. (12)+(13)]:

$$\mathbf{g}_{j(s+1)+i+1} \perp \widetilde{\mathbf{r}}_\ell^{(0)}, \quad 1 \leqslant \ell < i, \quad 0 \leqslant i \leqslant s, \quad j \geqslant 0, \tag{29a}$$

$$\mathbf{r}_{j(s+1)+i+1} \perp \widetilde{\mathbf{r}}_\ell^{(0)}, \quad 1 \leqslant \ell \leqslant i, \quad 0 \leqslant i \leqslant s, \quad j \geqslant 0. \tag{29b}$$

Here, to be consistent with [33], the first residual is $\mathbf{r}_1$, not $\mathbf{r}_0$. In addendum to [33] we set $\mathbf{g}_{j(s+1)+1} := -\mathbf{r}_{j(s+1)+1} \in \mathcal{G}_j$. The residual difference vectors $\mathbf{r}_{j(s+1)+i+1} - \mathbf{r}_{j(s+1)+i+2} \in \mathcal{G}_j$, $0 \leqslant i < s$, are used as new basis vector candidates, [33, p. 5:5]. The simple basis transformation induced by biorthogonality makes the algorithm easy to implement, as the small linear systems resulting from the projection become nested lower triangular, and the resulting Sonneveld pencils are usually better conditioned, i.e., the eigenvalue condition numbers of the Ritz values approximating eigenvalues of $\mathbf{A}$ first are mostly smaller than those obtained using IDR(s)ORes. Most Ritz values of the purified pencil are better conditioned than those of the Sonneveld or purified pencil of IDR(s)ORes.

Because of (29), the last residual in every cycle satisfies $\mathbf{v}_{j(s+1)} := \mathbf{r}_{j(s+1)} \in \mathcal{V}_{j-1}$, $j \geqslant 1$, thus for every choice of $\omega_j \neq 0$,

$$\mathbf{g}_{j(s+1)+1} = -\mathbf{r}_{j(s+1)+1} := -(\mathbf{I}_n - \omega_j \mathbf{A})\mathbf{r}_{j(s+1)} \in \mathcal{G}_j. \tag{30}$$

Since we construct $\mathbf{g}_{j(s+1)+i+1} \in \mathcal{G}_j$, $0 \leqslant i \leqslant s$, the remaining recurrences of "elegant" IDR(s) [33, p. 5:8], called IDR(s)BiO in [10], for $1 \leqslant i \leqslant s, j \geqslant 1$, can be restated as:

$$\begin{aligned}
\mathbf{v}_{j(s+1)+i} &:= \mathbf{r}_{j(s+1)+i} - \sum_{\ell=i}^{s} \mathbf{g}_{(j-1)(s+1)+\ell+1}\, \gamma_\ell^{(j(s+1)+i)} \in \mathcal{V}_{j-1}, \\
\mathbf{g}_{j(s+1)+i+1} &:= \mathbf{r}_{j(s+1)+i} - (\mathbf{I}_n - \omega_j \mathbf{A})\mathbf{v}_{j(s+1)+i} - \sum_{\ell=1}^{i-1} \mathbf{g}_{j(s+1)+\ell+1}\, \alpha_\ell^{(j(s+1)+i)} \\
&= \mathbf{A}\mathbf{v}_{j(s+1)+i}\, \omega_j + \sum_{\ell=i}^{s} \mathbf{g}_{(j-1)(s+1)+\ell+1}\, \gamma_\ell^{(j(s+1)+i)} \\
&\quad - \sum_{\ell=1}^{i-1} \mathbf{g}_{j(s+1)+\ell+1}\, \alpha_\ell^{(j(s+1)+i)} \in \mathcal{G}_j, \\
\mathbf{r}_{j(s+1)+i+1} &:= \mathbf{r}_{j(s+1)+i} - \mathbf{g}_{j(s+1)+i+1}\, \beta_i^{(j(s+1)+i)} \\
&= \mathbf{r}_{j(s+1)+1} - \sum_{\ell=1}^{i} \mathbf{g}_{j(s+1)+\ell+1}\, \beta_\ell^{(j(s+1)+\ell)} \in \mathcal{G}_j.
\end{aligned} \tag{31}$$

Here, the parameters γ, α, and β ensure $\mathbf{v}_{j(s+1)+i} \in \mathcal{V}_{j-1}$, the biorthogonality relations (29a) for the basis vectors, and the biorthogonality relations (29b) for the residual vectors, respectively. Removing the occurrences of $\mathbf{v}_{j(s+1)+i}$ and $\mathbf{r}_{j(s+1)+i}$ and sorting terms results in the columns

$$\mathbf{A}\Big(-\sum_{\ell=i}^{s}\mathbf{g}_{(j-1)(s+1)+\ell+1}\,\gamma_\ell^{(j(s+1)+i)}-\mathbf{g}_{j(s+1)+1}-\sum_{\ell=1}^{i-1}\mathbf{g}_{j(s+1)+\ell+1}\,\beta_\ell^{(j(s+1)+\ell)}\Big)\,\omega_j$$
$$=-\sum_{\ell=i}^{s}\mathbf{g}_{(j-1)(s+1)+\ell+1}\,\gamma_\ell^{(j(s+1)+i)}+\sum_{\ell=1}^{i-1}\mathbf{g}_{j(s+1)+\ell+1}\,\alpha_\ell^{(j(s+1)+i)}+\mathbf{g}_{j(s+1)+i+1} \tag{32}$$

with indices $j(s+1)+i$, $1\leqslant i\leqslant s$, of the generalized Hessenberg decomposition

$$\mathbf{A}\mathbf{G}_k\mathbf{U}_k^{\text{IDRBiO}}=\mathbf{G}_{k+1}\underline{\mathbf{H}}_k^{\text{IDRBiO}},\quad \mathbf{G}_{k+1}=\begin{pmatrix}\mathbf{G}_k & \mathbf{g}_{k+1}\end{pmatrix}=\begin{pmatrix}\mathbf{g}_1 & \cdots & \mathbf{g}_k & \mathbf{g}_{k+1}\end{pmatrix} \tag{33}$$

of IDRBiO. The missing columns with indices $j(s+1)$ result from Eq. (30):

$$\mathbf{A}\Big(-\mathbf{g}_{(j-1)(s+1)+1}-\sum_{\ell=1}^{s}\mathbf{g}_{(j-1)(s+1)+\ell+1}\,\beta_\ell^{((j-1)(s+1)+\ell)}\Big)\,\omega_j$$
$$=-\mathbf{g}_{(j-1)(s+1)+1}-\sum_{\ell=1}^{s}\mathbf{g}_{(j-1)(s+1)+\ell+1}\,\beta_\ell^{((j-1)(s+1)+\ell)}+\mathbf{g}_{j(s+1)}. \tag{34}$$

The shape of the extended Sonneveld pencil $(\underline{\mathbf{H}}_k^{\text{IDRBiO}},\mathbf{U}_k^{\text{IDRBiO}})$ of IDRBiO looks similar to that of IDROREs, apart from additional zero patterns of s consecutive zeros in the rows $j(s+1)$, $j\geqslant 1$. The IDR parameters γ enter both the upper triangular parts of $\underline{\mathbf{H}}_k^{\text{IDRBiO}}$ and $\mathbf{U}_k^{\text{IDRBiO}}$, the biorthogonalization parameters β for the residual vectors only $\mathbf{U}_k^{\text{IDRBiO}}$, and the biorthogonalization parameters α for the basis vectors only $\underline{\mathbf{H}}_k^{\text{IDRBiO}}$. The parameters ω_j again are applied only in forming $\mathbf{U}_k^{\text{IDRBiO}}$ and result in known eigenvalues $1/\omega_j$ of the square Sonneveld pencil $(\mathbf{H}_k^{\text{IDRBiO}},\mathbf{U}_k^{\text{IDRBiO}})$ for every completed ω_j-block. The Sonneveld pencil of IDRBiO can and should be purified and deflated like in case of IDROREs.

4.3. IDR(s)Stab(ℓ) *[11, 13]*

In IDRStab the aim is to combine the advantages of the higher dimensional shadow spaces in IDR(s) with those of the higher dimensional minimization in BiCGStab(ℓ). In IDRStab, IDR vectors are computed along with purified Lanczos vectors up to the IDR step $k(\ell+1)$, where a (modified) GMRes polynomial Γ_k of degree ℓ is computed; then everything is repeated on a higher level with vectors that have as a common factor the product of all Γ-polynomials constructed so far. In IDRStab, before the polynomial step, *many* different generalized Hessenberg decompositions along with the corresponding pencils can be defined, the most important ones are the *full* IDRStab *pencil*, useful in the error analysis, and the *Lanczos*-IDRStab *pencil*, useful in eigenvalue computations [37].

To understand IDRStab, thinking in terms of a *Hessenberg scheme* of matrices and vectors, see Eq. (37), simplifies the derivation of the generalized Hessenberg decompositions and the corresponding pencils. In Sleijpen's implementation, the following Sonneveld spaces are involved in the computation of the columns of the matrices in the diagonal of the Hessenberg scheme (37):

$$\begin{aligned}\mathcal{G}_{k(\ell+1)+i}&:=\mathcal{S}(m_i\,\Gamma_k\cdots\Gamma_2\Gamma_1,\mathbf{A},\widetilde{\mathbf{R}}_0),\\ \mathcal{V}_{k(\ell+1)+i}&:=\mathcal{G}_{k(\ell+1)+i}\cap\mathcal{S},\end{aligned}\qquad k\geqslant 0,\quad 0\leqslant i\leqslant\ell. \tag{35}$$

Here, $k\geqslant 0$ denotes the kth cycle of IDRStab and $m_i(z):=z^i$ denotes the ith monomial function, e.g., the first space is given by $\mathcal{G}_0=\mathcal{K}=\mathcal{K}_n(\mathbf{A},\mathbf{r}_0)$ as before, and apart from $\mathcal{G}_{k(\ell+1)}$ for $k>1$, we mostly use the "traditional" update well known for the IDR spaces,

$$\mathcal{G}_{k(\ell+1)+i+1}=\mathbf{A}(\mathcal{G}_{k(\ell+1)+i}\cap\mathcal{S})=\mathbf{A}\mathcal{V}_{k(\ell+1)+i},\quad k\geqslant 0,\quad 0\leqslant i<\ell. \tag{36}$$

We stress the fact that the index of the left block Krylov subspace is given by the degree $k\ell+i$ of the polynomial defining the Sonneveld space, i.e., the *order* of the Sonneveld space [13, Defin-

ition 2.2], and thus mostly does not correspond to the index $k(\ell+1)+i$ of the space $\mathcal{G}_{k(\ell+1)+i}$ constructed. In the kth cycle of IDRStab, the following matrices $\mathbf{G}_{i,j}^{(k)} \in \mathbb{C}^{n\times s}$ and vectors $\mathbf{r}_{i,j}^{(k)} \in \mathbb{C}^n$ are computed:

$$\underline{\mathfrak{H}}_k := \begin{pmatrix} \mathbf{G}_{1,1}^{(k)}, \mathbf{r}_{1,1}^{(k)} & \mathbf{G}_{1,2}^{(k)}, \mathbf{r}_{1,2}^{(k)} & \dots & \mathbf{G}_{1,\ell}^{(k)}, & \mathbf{r}_{1,\ell}^{(k)} & \mathbf{G}_{1,\ell+1}^{(k)}, \mathbf{r}_{1,\ell+1}^{(k)} \\ \mathbf{G}_{2,1}^{(k)}, \mathbf{r}_{2,1}^{(k)} & \mathbf{G}_{2,2}^{(k)}, \mathbf{r}_{2,2}^{(k)} & \dots & \mathbf{G}_{2,\ell}^{(k)}, & \mathbf{r}_{2,\ell}^{(k)} & \mathbf{G}_{2,\ell+1}^{(k)} \\ & \mathbf{G}_{3,2}^{(k)}, \mathbf{r}_{3,2}^{(k)} & \ddots & \vdots & & \vdots \\ & & \ddots & \mathbf{G}_{\ell,\ell}^{(k)}, & \mathbf{r}_{\ell,\ell}^{(k)} & \mathbf{G}_{\ell,\ell+1}^{(k)} \\ & & & \mathbf{G}_{\ell+1,\ell}^{(k)}, & \mathbf{r}_{\ell+1,\ell}^{(k)} & \mathbf{G}_{\ell+1,\ell+1}^{(k)} \\ & & & & & \mathbf{G}_{\ell+2,\ell+1}^{(k)} \end{pmatrix} \in \mathbb{C}^{(\ell+2)n\times(s+1)(\ell+1)}, \quad (37)$$

here,

$$\begin{aligned} &\mathbf{G}_{i,i}^{(k)} \ , \mathbf{r}_{i,i}^{(k)} \ \in \mathcal{G}_{k(\ell+1)+i-1}, \quad 1 \leqslant i \leqslant \ell+1, \\ &\mathbf{G}_{i,i}^{(k)} \ , \mathbf{r}_{i,i}^{(k)} \ \in \mathcal{V}_{k(\ell+1)+i-1}, \quad 2 \leqslant i \leqslant \ell+1, \qquad \mathbf{r}_{1,1}^{(k)} \in \mathcal{V}_{k(\ell+1)}, \\ &\mathbf{G}_{i+1,i}^{(k)}, \mathbf{r}_{i+1,i}^{(k)} \in \mathcal{G}_{k(\ell+1)+i} \quad , \quad 2 \leqslant i \leqslant \ell \qquad , \end{aligned} \quad (38)$$

where, with abuse of notation, $\mathbf{G}_{i,i}^{(k)} \in \mathcal{G}_{k(\ell+1)+i-1}$ is shorthand for $\mathbf{G}_{i,i}^{(k)}\mathbf{e}_1, \dots, \mathbf{G}_{i,i}^{(k)}\mathbf{e}_s \in \mathcal{G}_{k(\ell+1)+i-1}$. The relations $\mathbf{G}_{i+1,j}^{(k)} = \mathbf{A}\mathbf{G}_{i,j}^{(k)}$ and $\mathbf{r}_{i+1,j}^{(k)} = \mathbf{A}\mathbf{r}_{i,j}^{(k)}$, $1 \leqslant i \leqslant j$, are forced by construction. These allow to move inside the columns of the Hessenberg scheme (37) by synthetically multiplying with or dividing by $\mathbf{A}$; this is used for the manipulation of the mathematical relations defining IDRStab. In simple IDR(s) methods only the *diagonal* of this scheme would be computed; in IDRStab additional sets of vectors are computed, which are necessary to complete the polynomial step. The freedom in choosing the basis vectors is fixed in [13] by computing orthonormal blocks $\mathbf{G}_{ii}^{(k)}$, $2 \leqslant i \leqslant \ell+1$, i.e., most matrices in the diagonal of the scheme are orthonormal.

Initialization is done using Arnoldi's method which defines the first block column of the Hessenberg scheme (37) along with an extended Hessenberg matrix $\underline{\mathbf{H}}_{s-1}^{(0)} \in \mathbb{C}^{s\times(s-1)}$ containing the orthonormalization constants,

$$\mathbf{G}_{1,1}^{(0)}\mathbf{e}_1 := \mathbf{r}_0/\|\mathbf{r}_0\|_2, \quad \mathbf{G}_{2,1}^{(0)} := \mathbf{A}\mathbf{G}_{1,1}^{(0)} = \begin{pmatrix} \mathbf{G}_{1,1}^{(0)} & \mathbf{G}_{2,1}^{(0)}\mathbf{e}_s \end{pmatrix} \begin{pmatrix} \underline{\mathbf{H}}_{s-1}^{(0)} & \mathbf{o}_s \\ \mathbf{o}_{s-1}^{\mathsf{T}} & 1 \end{pmatrix}. \quad (39)$$

The computation of the elements of the Hessenberg scheme (37) evolves along the diagonal and updates columnwise. The first primary residual $\mathbf{r}_{1,1}^{(0)}$ of IDRStab is computed by oblique projection using $\mathbf{G}_{2,1}^{(0)} = \mathbf{A}\mathbf{G}_{1,1}^{(0)}$ [13, Eqs. (5.3)+(5.4)],

$$\begin{aligned} \mathbf{r}_{1,1}^{(0)} &:= \mathbf{r}_0 - \mathbf{G}_{2,1}^{(0)}\alpha_1^{(0)} := (\mathbf{I} - \mathbf{G}_{2,1}^{(0)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{2,1}^{(0)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_0 \in \mathcal{V}_0 \\ &= \mathbf{r}_0 - \mathbf{A}\mathbf{G}_{1,1}^{(0)}\alpha_1^{(0)} = \mathbf{G}_{1,1}^{(0)}\mathbf{e}_1\|\mathbf{r}_0\|_2 - \mathbf{A}\mathbf{G}_{1,1}^{(0)}\alpha_1^{(0)}, \quad \mathbf{r}_{2,1}^{(0)} := \mathbf{A}\mathbf{r}_{1,1}^{(0)} \in \mathcal{G}_1. \end{aligned} \quad (40)$$

The diagonal blocks $\mathbf{G}_{i,i}^{(k)}$, $2 \leqslant i \leqslant \ell+1$ for $k \geqslant 0$, are updated as described in [13, Section 5.1] and are orthonormalized for enhanced stability, see [13, Section 5.4],

$$\begin{aligned}
\mathbf{G}_{i,i}^{(k)}\mathbf{e}_1 &:= (\mathbf{r}_{i,i-1}^{(k)} - \mathbf{G}_{i,i-1}^{(k)}\beta_{i-1}^{(k)}\mathbf{e}_1)/h_{1,1}^{(k,i)} \\
&= \mathbf{A}(\mathbf{r}_{i-1,i-1}^{(k)} - \mathbf{G}_{i-1,i-1}^{(k)}\beta_{i-1}^{(k)}\mathbf{e}_1)/h_{1,1}^{(k,i)}, \quad \mathbf{G}_{i+1,i}^{(k)}\mathbf{e}_1 := \mathbf{A}\mathbf{G}_{i,i}^{(k)}\mathbf{e}_1, \\
\mathbf{G}_{i,i}^{(k)}\mathbf{e}_{j+1} &:= \Big(\mathbf{G}_{i+1,i}^{(k)}\mathbf{e}_j - \mathbf{G}_{i,i-1}^{(k)}\beta_{i-1}^{(k)}\mathbf{e}_j - \sum_{\eta=1}^{j}\mathbf{G}_{i,i}^{(k)}\mathbf{e}_\eta h_{\eta,j+1}^{(k,i)}\Big)/h_{j+1,j+1}^{(k,i)} \\
&= \mathbf{A}\Big(\mathbf{G}_{i,i}^{(k)}\mathbf{e}_j - \mathbf{G}_{i-1,i-1}^{(k)}\beta_{i-1}^{(k)}\mathbf{e}_j\Big)/h_{j+1,j+1}^{(k,i)} \\
&\quad - \left(\sum_{\eta=1}^{j}\mathbf{G}_{i,i}^{(k)}\mathbf{e}_\eta h_{\eta,j+1}^{(k,i)}\right)/h_{j+1,j+1}^{(k,i)}, \quad 1 \leqslant j < s, \\
\mathbf{G}_{i+1,i}^{(k)}\mathbf{e}_{j+1} &:= \mathbf{A}\mathbf{G}_{i,i}^{(k)}\mathbf{e}_{j+1}, \quad 1 \leqslant j < s.
\end{aligned} \tag{41}$$

Here, the columns of $\beta_i^{(k)} \in \mathbb{C}^{s\times s}$, $1 \leqslant i \leqslant \ell$, are chosen such that the result is contained in $\mathcal{S}$, and the upper triangular matrix $\mathbf{H}_s^{(k,i)} \in \mathbb{C}^{s\times s}$ contains the orthonormalization parameters that ensure that $\mathbf{G}_{i,i}^{(k)}$ is orthonormal. The (partially) purified basis vectors $\mathbf{G}_{j,i}^{(k)}$, $1 \leqslant j < i$ are obtained using synthetic division and result in similar update formulæ for the other matrices in the same column.

For $k \geqslant 0$, $2 \leqslant i \leqslant \ell$, the update of the vectors $\mathbf{r}_{i,i}^{(k)}$ in the diagonal proceeds as follows,

$$\begin{aligned}
\mathbf{r}_{i,i}^{(k)} &:= \mathbf{r}_{i,i-1}^{(k)} - \mathbf{G}_{i+1,i}^{(k)}\alpha_i^{(k)} := (\mathbf{I} - \mathbf{G}_{i+1,i}^{(k)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{i+1,i}^{(k)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_{i,i-1}^{(k)} \\
&= \mathbf{A}(\mathbf{r}_{i-1,i-1}^{(k)} - \mathbf{G}_{i,i}^{(k)}\alpha_i^{(k)}) \in \mathcal{V}_{k(\ell+1)+i-1}, \quad \mathbf{r}_{i+1,i}^{(k)} := \mathbf{A}\mathbf{r}_{i,i}^{(k)}.
\end{aligned} \tag{42}$$

The (partially) purified vectors $\mathbf{r}_{j,i}^{(k)}$, $1 \leqslant j < i$ are obtained using synthetic division,

$$\mathbf{r}_{j,i}^{(k)} := \mathbf{r}_{j,i-1}^{(k)} - \mathbf{G}_{j+1,i}^{(k)}\alpha_i^{(k)}, \quad 1 \leqslant j < i. \tag{43}$$

We remark that before the polynomial step occurs, IDRStab returns the Lanczos$(s, 1)$ residuals $\mathbf{r}_{i,1}^{(0)}$, $1 \leqslant i \leqslant \ell$, as primary residuals, compare with TFIQMR [27]; to our knowledge the computation of Lanczos$(s, 1)$ quantities was first used in the IDR(s) context in [10].

In the polynomial step,

$$\mathbf{r}_{1,\ell+1}^{(k)} := \mathbf{r}_{1,\ell}^{(k)} - \sum_{i=1}^{\ell}\mathbf{r}_{i+1,\ell}^{(k)}\gamma_i^{(k)}, \qquad \begin{aligned}\mathbf{G}_{1,1}^{(k+1)} &:= \mathbf{G}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell}\mathbf{G}_{i+1,\ell+1}^{(k)}\gamma_i^{(k)}, \\ \mathbf{G}_{2,1}^{(k+1)} &:= \mathbf{G}_{2,\ell+1}^{(k)} - \sum_{i=1}^{\ell}\mathbf{G}_{i+2,\ell+1}^{(k)}\gamma_i^{(k)},\end{aligned} \tag{44}$$

i.e., $\mathbf{r}_{1,\ell+1}^{(k)} = \Gamma_k(\mathbf{A})\,\mathbf{r}_{1,\ell}^{(k)}$, $\mathbf{G}_{1,1}^{(k+1)} = \Gamma_k(\mathbf{A})\,\mathbf{G}_{1,\ell+1}^{(k)}$, $\mathbf{G}_{2,1}^{(k+1)} = \Gamma_k(\mathbf{A})\,\mathbf{G}_{2,\ell+1}^{(k)}$, where the polynomial Γ_k defined by $\Gamma_k(z) := 1 - \sum_{i=1}^{\ell}\gamma_i^{(k)}z^i$, is either a GMRes residual polynomial, or a modification thereof, as sketched in [38,13]. By construction, $\mathbf{G}_{2,1}^{(k+1)} = \mathbf{A}\mathbf{G}_{1,1}^{(k+1)}$.

Up to step $\ell+1$, several generalized Hessenberg decompositions can be defined. The so-called IDR-IDRStab generalized Hessenberg decomposition captures the IDR variant that builds up the diagonal of the Hessenberg scheme (37) and is given by

$$\mathbf{A}\mathbf{G}_{(\ell+1)(s+1)-2}^{\text{IDR}}\mathbf{U}_{(\ell+1)(s+1)-2}^{\text{IDR-IDRStab}} = \mathbf{G}_{(\ell+1)(s+1)-1}^{\text{IDR}}\underline{\mathbf{H}}_{(\ell+1)(s+1)-2}^{\text{IDR-IDRStab}}, \tag{45}$$

where with $\nu := (\ell+1)(s+1)-2$,

$$\begin{aligned}
\mathbf{G}^{\text{IDR}}_{(\ell+1)(s+1)-1} &:= \left(\mathbf{G}^{\text{IDR}}_{(\ell+1)(s+1)-2}\ \mathbf{g}^{\text{IDR}}_{(\ell+1)(s+1)-1}\right)\\
&:= \left(\mathbf{G}^{(0)}_{1,1}\ \mathbf{r}^{(0)}_{1,1}\ \mathbf{G}^{(0)}_{2,2}\ \mathbf{r}^{(0)}_{2,2}\ \cdots\ \mathbf{G}^{(0)}_{\ell+1,\ell+1}\right) \in \mathbb{C}^{n\times(\nu+1)},\\
\mathbf{U}^{\text{IDR-IDRStab}}_{(\ell+1)(s+1)-2} &:= \begin{pmatrix}
\underline{\mathbf{I}}_{s-1} & \alpha_1^{(0)} & -\beta_1^{(0)} & & & & & & & \\
 & & & -1 & \mathbf{o}_s^{\mathsf{T}} & & & & & \\
 & & \underline{\mathbf{I}}_s & \alpha_2^{(0)} & -\beta_2^{(0)} & & & & & \\
 & & & & & -1 & \mathbf{o}_s^{\mathsf{T}} & & & \\
 & & & & \underline{\mathbf{I}}_s & \alpha_3^{(0)} & -\beta_3^{(0)} & & & \\
 & & & & & & \underline{\mathbf{I}}_s & \ddots & & \\
 & & & & & & & \ddots & \mathbf{o}_s^{\mathsf{T}} & \\
 & & & & & & & & -\beta_\ell^{(0)} & \\
 & & & & & & & & \mathbf{I}_s &
\end{pmatrix} \in \mathbb{C}^{\nu\times\nu},\\
\underline{\mathbf{H}}^{\text{IDR-IDRStab}}_{(\ell+1)(s+1)-2} &:= \begin{pmatrix}
\underline{\mathbf{H}}^{(0)}_{s-1} & \mathbf{e}_1\|\mathbf{r}_0\|_2 & & & & \\
\mathbf{o}_{s-1}^{\mathsf{T}} & -1 & & & & \\
 & & \mathbf{H}^{(1)}_s & & & \\
 & & & -1 & & \\
 & & & & \ddots & \\
 & & & & & \mathbf{H}^{(\ell)}_s
\end{pmatrix} \in \mathbb{C}^{(\nu+1)\times\nu}.
\end{aligned} \tag{46}$$

The undeflated Lanczos-IDRStab generalized Hessenberg decomposition is obtained by purifying the polynomials defining the IDR vectors, i.e., the columns of $\mathbf{G}^{\text{IDR}}_{(\ell+1)(s+1)-1}$, from the consecutive powers of $\mathbf{A}$ and is given by

$$\mathbf{A}\mathbf{G}^{\text{Lanczos}}_{(\ell+1)(s+1)-2}\mathbf{U}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-2} = \mathbf{G}^{\text{Lanczos}}_{(\ell+1)(s+1)-1}\underline{\mathbf{H}}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-2}, \tag{47}$$

where the matrices are defined by:

$$\begin{aligned}
\mathbf{G}^{\text{Lanczos}}_{(\ell+1)(s+1)-1} &:= \left(\mathbf{G}^{\text{Lanczos}}_{(\ell+1)(s+1)-2}\ \mathbf{g}^{\text{Lanczos}}_{(\ell+1)(s+1)-1}\right)\\
&:= \left(\mathbf{G}^{(0)}_{1,1}\ \mathbf{r}^{(0)}_{1,1}\ \mathbf{G}^{(0)}_{1,2}\ \mathbf{r}^{(0)}_{1,2}\ \cdots\ \mathbf{G}^{(0)}_{1,\ell+1}\right) \in \mathbb{C}^{n\times(\nu+1)},\\
\mathbf{U}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-2} &:= \begin{pmatrix}
\underline{\mathbf{I}}_{s-1} & \alpha_1^{(0)} & & & & & & \\
 & 0 & & & & & & \\
 & \underline{\mathbf{I}}_{s-1} & \alpha_2^{(0)} & & & & & \\
 & & & \ddots & & & & \\
 & & & & 0 & & & \\
 & & & & \underline{\mathbf{I}}_{s-1} & \alpha_\ell^{(0)} & & \\
 & & & & & 0 & & \\
 & & & & & & \mathbf{I}_{s-1} &
\end{pmatrix} \in \mathbb{C}^{\nu\times\nu},
\end{aligned} \tag{48}$$

$$\underline{\mathbf{H}}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-2} := \begin{pmatrix} \underline{\mathbf{H}}^{(0)}_{s-1} & \mathbf{e}_1\|\mathbf{r}_0\|_2 & \beta^{(0)}_1 & \mathbf{o}_s & & & & & \\ \mathbf{o}^\top_{s-1} & -1 & -\mathbf{e}^\top_1 & 1 & & & & & \\ & & \mathbf{H}^{(1)}_s & \mathbf{o}_s & \ddots & & & & \\ & & \mathbf{o}^\top_s & -1 & & & & & \\ & & & & \ddots & \beta^{(0)}_{\ell-1} & \mathbf{o}_s & & \\ & & & & & -\mathbf{e}^\top_1 & 1 & & \\ & & & & & \mathbf{H}^{(\ell)}_s & \mathbf{o}_s & \beta^{(0)}_\ell & \\ & & & & & \mathbf{o}^\top_s & -1 & -\mathbf{e}^\top_1 & \\ & & & & & & & \mathbf{H}^{(\ell+1)}_s & \end{pmatrix} \in \mathbb{C}^{(\nu+1)\times\nu}. \tag{49}$$

Since the IDR variant driving IDRStab is based solely on multiplication with $\mathbf{A}$, the purification simply moves the β-blocks and some plus and minus ones from the upper triangular $\mathbf{U}^{\text{IDR-IDRStab}}_{(\ell+1)(s+1)-2}$ to the upper Hessenberg $\mathbf{H}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-2}$. The resulting $\mathbf{U}^{\text{Lanczos-IDRStab}}_{(\ell+1)(s+1)-1}$ is singular, which is reflected in the ℓ *infinite* eigenvalues of the Lanczos-IDRStab pencil that replace the ℓ known *zero* eigenvalues of the IDR-IDRStab pencil.

There exist in total 2^ℓ generalized Hessenberg decompositions together with corresponding pencils describing the various paths in the Hessenberg scheme (37): after every IDR step we can either multiply with $\mathbf{A}$ and move in diagonal direction, or omit the multiplication with $\mathbf{A}$ and stay in that row. None of these pencils can easily be extended beyond the polynomial step, even though the diagonal elements of the scheme (37) build a basis of $\mathcal{G}_0 = \mathcal{K}$ provided no breakdown or deflation occurs. The reason is that the linear combination is along the last *column* of the scheme (37), thus we need either some algebraic transformations, or access to all the $\mathbf{G}$-blocks in that column. One solution is the *full* IDRStab pencil that describes all the blocks in the upper triangular of the Hessenberg scheme (37). We do not discuss the full IDRStab pencil here.

As all the pencils contain the same eigenvalue information apart from zero or infinite eigenvalues due to the nature of Sonneveld methods and multiplication with $\mathbf{A}$ corresponding to the monomial $m_1(z) = z$ with the only root zero, we use the Lanczos-IDRStab pencil that only has additional infinite eigenvalues. Even though we do not have the corresponding basis vectors, we can easily extend the pencil beyond the polynomial step and obtain a purified pencil in *every* step of IDRStab. This pencil can also be deflated to obtain the upper Hessenberg block-tridiagonal matrix of the underlying Lanczos$(s, 1)$ process.

4.4. A numerical comparison

All numerical experiments were carried out using Matlab 7.14.0.739 (R2012a) on a 64bit Arch Linux Laptop with Linux Kernel 3.3.1. We used the matrix `e05r0500` and corresponding right-hand side `e05r0500_rhs1` from the Matrix Market with zero initial guess. The reason to use a right-hand side in an eigenvalue computation is that in this way we ensure to have a physically meaningful mixture of eigenvectors in the starting vector. We tested the behavior of the three algorithms for eigenvalue approximation, the parameters were chosen identical, e.g., we used the same $\widetilde{\mathbf{R}}_0$. We always used a purified pencil and Matlab's `eig`.

In Fig. 1 we plotted the distances of the closest Ritz values of the purified pencils to the outlier $\lambda \approx 4.2505 + 44.2719i$ computed with `eig` for $s = 6$. By nature of IDR, all these curves should intersect every $s+1 = 7$ steps. IDR(6)ORes is based on OrthoRes(1) in the first steps, thus the first six approximations are pretty bad. IDR(6)ORes is the most unstable method, IDR(6)BiO and IDR(6)Stab(ℓ) are quite similar and show better convergence properties. Increasing the polynomial degree gives worse convergence behavior, we suggest to use $\ell = 1$ or $\ell = 2$. The plot shows the average behavior of these methods, except for IDR(6)BiO: the oscillations at the end came up roughly every seventh

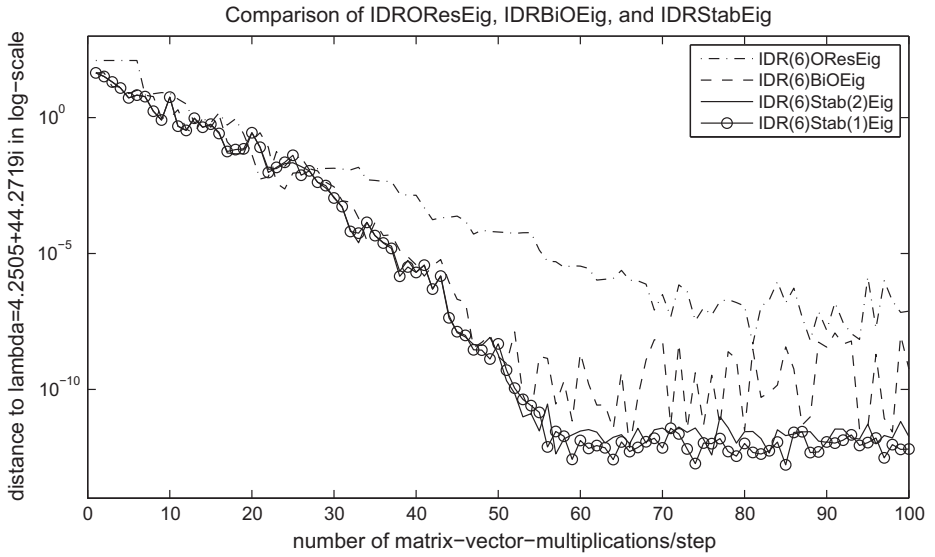

Fig. 1. Comparison of the eigenvalue approximation behavior of IDR(6)ORes, IDR(6)BiO, IDR(6)Stab(2) and IDR(6)Stab(1).

run when a random orthonormal $\widetilde{\mathbf{R}}_0$ was chosen. The methods based on (bi)orthonormalization are clearly superior in this example.

4.5. A thought experiment

Sonneveld methods have the power to bridge between Lanczos's and Arnoldi's method, compare with [14], where this statement is analyzed for the linear system case with Arnoldi's method replaced by GMRes. In the eigenvalue counterpart, a similar observation can be made. In Fig. 2 we present a supporting example based on the same data as in the previous subsection.

We count every matrix–vector multiplication, i.e., in Lanczos's method we count the multiplication with $\mathbf{A}$ and with $\mathbf{A}^{\mathsf{H}}$ separately, thus we obtain a new Ritz value every other step. As IDR method we used IDRStab with $\ell = 1$, as this seems to be the stablest method of the three methods considered. We used the first columns of one random orthonormal matrix as shadow vectors $\widetilde{\mathbf{R}}_0$ or left starting vector. Lanczos's method is mathematically equivalent with the purified recurrence of IDR(1), which is clearly visible up to step 40. Afterwards, the two methods return different approximations due to finite precision issues. Increasing the value of s gives mostly a steeper convergence curve, i.e., the four IDR curves are clearly distinguishable despite we used the same line type. Already the convergence curve of IDR(6) is pretty close to the curve resulting from Arnoldi's method, the curve of IDR(24) only slightly improves at the expense of much more memory necessary in the course of computation.

4.6. Towards a genuine IDR-based eigensolver

In order to compute good approximations to eigenvalues we need a stable basis represented by $\mathbf{G}_k$. The numerical experiments lead us to the conclusion that choosing $\mathbf{G}_k$ 'as orthonormal as possible' is a good idea. Based on experiments with structured $\widetilde{\mathbf{R}}_0$ we mostly use orthonormalized random vectors. A high degree of the stabilizing polynomials, which are deflated in any case in the eigenvalue solvers, makes the methods more unstable. The choice of roots of these stabilizing polynomials has to be done carefully, as finite precision effects result in sometimes surprising behavior. Common in all IDR methods tested is the occurrence of past polynomial roots as spurious Ritz values in later iterations. We had good experiences with the ideas presented in [38,13], but Rayleigh quotients with vectors from the recurrence also seem promising.

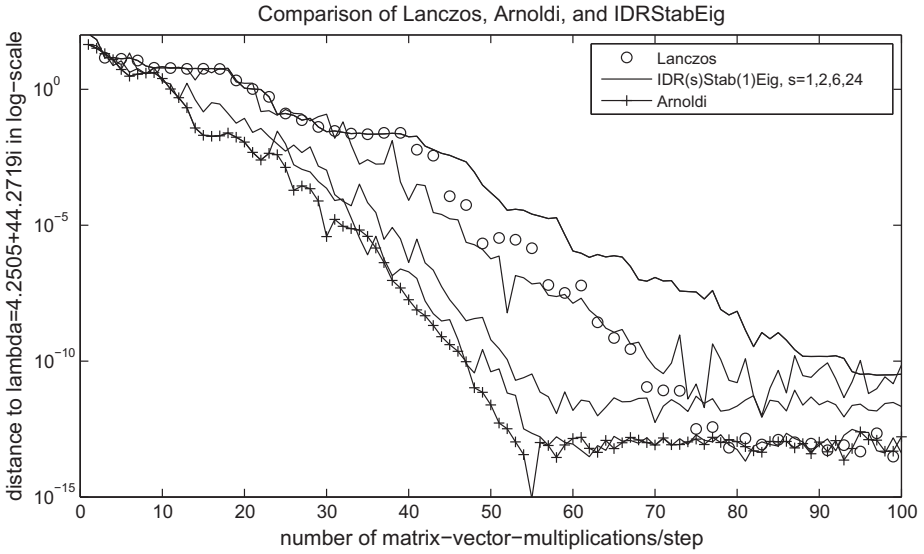

Fig. 2. Comparison of Lanczos's method, Sonneveld methods for varying s ($s = k!$ for $k = 1, \ldots, 4$), and Arnoldi's method. The starting vectors have been chosen such that Lanczos's method is mathematically equivalent with IDR(1).

5. Solution of linear systems

There are many IDR based methods for the approximate solution of linear systems: IDRORes or prototype IDR(s) [1], soon superseded by IDRBiO [33], which uses a bi-orthogonalization scheme for stability reasons, and the generalization IDRStab [11,13] allowing for incorporation of stabilizing polynomials of degree larger than one. All these methods are of type OR. Methods of type MR are more recent [15,32]. We remark that the well-known peak-plateau phenomenon discussed in [39] carries over to the corresponding pairs of OR and MR Sonneveld methods, as the coefficient vectors $\mathbf{z}_k$ and $\underline{\mathbf{z}}_k$ are defined completely analogous, the difference to classical Krylov subspace methods lies in the basis used, i.e., $\mathbf{V}_k = \mathbf{G}_k\mathbf{U}_k$ replaces $\mathbf{G}_k$. Mathematically, the MR variant of a given OR variant can be obtained by smoothing [35]; in finite precision MR variants resulting from smoothing are not competitive with direct implementations of the MR approach, cf. [32]. Within the framework of generalized Hessenberg decompositions and relations it is easy to derive flexible and multi-shift variants [32].

In the next subsection we sketch an important peculiarity of IDR methods related to breakdown of OR and stagnation of MR. Further subsections are devoted to the choices of a 'good' basis, the 'stabilizing' polynomials, and the shadow space.

5.1. Breakdown and stagnation

In classical Krylov subspace methods the occurrence of a singular Hessenberg matrix results in a temporary breakdown of the OR approach and a stagnation of the corresponding MR approach. In contrast, in IDR based methods there is the additional possibility of an *absolute breakdown* of the OR approach and an *infinite stagnation* of the MR approach. This is even more pronounced in multi-shift methods:

Lemma 3 (Absolute breakdown and infinite stagnation in IDR)**.** *Suppose we solve a sequence of shifted systems* $(\mathbf{A} - \sigma\mathbf{I})\mathbf{x}^\sigma = \mathbf{r}_0$ *with an IDR method captured by the family of generalized Hessenberg decompositions*

$$(\mathbf{A}-\sigma\mathbf{I})\mathbf{V}_k = (\mathbf{A}-\sigma\mathbf{I})\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}(\underline{\mathbf{H}}_k-\sigma\underline{\mathbf{U}}_k) =: \mathbf{G}_{k+1}\underline{\mathbf{H}}_k^{(\sigma)} = \mathbf{G}_k\mathbf{H}_k^{(\sigma)}+\mathbf{g}_{k+1}h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}. \quad (50)$$

If in step k_∞ a new root of a stabilizing polynomial is equal to a shift σ, all Hessenberg matrices $\mathbf{H}_k^{(\sigma)}$, $k \geqslant k_\infty$, will be singular, i.e., the OR approach has an absolute breakdown, and the MR approach suffers from infinite stagnation.

Proof. By nature of Krylov subspace methods we know that $\mathbf{g}_{k+1} = g_k(\mathbf{A})\mathbf{r}_0$ for some polynomial g_k. By nature of IDR methods, i.e., utilizing the description of the Sonneveld spaces (5), this polynomial has the product of all previous stabilizing polynomials as a factor.[7] In [10, Theorem 2.2] it is proven that the basis vectors corresponding to a generalized Hessenberg decomposition satisfy $g_k(z) = \det(z\mathbf{U}_k - \mathbf{H}_k)/(\|\mathbf{r}_0\| \cdot \prod_{\ell=1}^{k} h_{\ell+1,\ell})$. Thus, $g_k(\nu) = 0$, $k \geqslant k_\infty$ for all roots ν of the stabilizing polynomial chosen to compute $\mathbf{g}_{k_\infty+1}$. This implies that $\det(\mathbf{H}_k - \nu\mathbf{U}_k)$ is zero, $k \geqslant k_\infty$, and thus, for $\sigma = \nu$, that $\mathbf{H}_k^{(\sigma)} = \mathbf{H}_k - \sigma\mathbf{U}_k$ is singular, $k \geqslant k_\infty$. □

This lemma is easily applicable in case of given shifts (e.g., the only shift $\sigma = 0$, i.e., no multi-shift at all), or in IDR methods that rely on linear polynomials, i.e., excluding IDRStab. Similar to other types of breakdown, the roots should not be chosen "too close" to the shifts (zero). A precise interpretation of "too close" still has to be determined and a scheme for choosing the roots still has to be developed. Especially, the adaption of ideas to multi-shift variants appears to be non-straightforward. The sensitivity of IDR methods at the roots of the stabilizing polynomials is reflected in the numerical experiments; we observed for all the methods considered spurious Ritz values close to the previously used roots.

5.2. Choice of the basis

There is some freedom in the construction of the basis vectors $\mathbf{g}$; we can use linear combinations with previously computed vectors in the same space in every new space $\mathcal{G}_j$. A natural and old idea is to use the OR residuals as basis vectors, as these are always parallel to the basis vectors. This is done in IDRORes [1] and in the QMRIDR variant [15] based on it. Unfortunately, this approach is known to suffer from instabilities when zero is in the field of values of $\mathbf{A}$ and should not be used. Using the MR approach does not improve, as the basis itself is not stable.

More stable approaches are based on a partial orthonormalization of the basis vectors, like in Sleijpen's implementation of IDRStab [13] or the QMRIDR variant [32]. These methods usually work better than the others, especially for larger values of s, and frequently result in a lower level of ultimately attainable accuracy. This can also be observed when these methods are used as eigenvalue solvers, as sketched in Section 4. Apart from an increased stability in the numerical experiments, we can also derive a better bound on the true residual. Our following result can originally be found in [32]:

Lemma 4 (Norm of a block-wise orthonormal matrix)**.** *Suppose $\mathbf{G}_{k+1} = (\mathbf{G}^{(1)}, \ldots, \mathbf{G}^{(j)})$, where $\mathbf{G}^{(\ell)}$ is orthonormal, $1 \leqslant \ell \leqslant j$.*

Then

$$\|\mathbf{G}_{k+1}\| \leqslant \sqrt{j}. \tag{51}$$

Proof. Partition $\mathbf{w} \in \mathbb{C}^{k+1}$ block-wise into vectors $\mathbf{w}_\ell$ conforming with the sizes of the blocks $\mathbf{G}^{(\ell)}$, $1 \leqslant \ell \leqslant j$, i.e., $\mathbf{G}_{k+1}\mathbf{w} = \sum_{\ell=1}^{j} \mathbf{G}^{(\ell)}\mathbf{w}_\ell$. Then

$$\begin{aligned} \|\mathbf{G}_{k+1}\|^2 &= \max_{\|\mathbf{w}\|^2=1} \|\mathbf{G}_{k+1}\mathbf{w}\|^2 = \max_{\|\mathbf{w}\|^2=1} \Big\|\sum_{\ell=1}^{j} \mathbf{G}^{(\ell)}\mathbf{w}_\ell\Big\|^2 \\ &\leqslant \sum_{\ell=1}^{j} \max_{\|\mathbf{w}_\ell\|^2=1} \|\mathbf{G}^{(\ell)}\mathbf{w}_\ell\|^2 = \sum_{\ell=1}^{j} \max_{\|\mathbf{w}_\ell\|^2=1} \|\mathbf{w}_\ell\|^2 = \sum_{\ell=1}^{j} 1 = j. \end{aligned} \tag{52}$$

[7] More precisely: it can be written as a product of two polynomials, namely, the product of all previous stabilizing polynomials and a Lanczos$(s, 1)$ polynomial, compare with the special case treated in [10].

Taking square roots proves the lemma. □

5.3. Choice of the stabilizing polynomials

In this subsection, we do not consider multi-shift variants. By Lemma 3 we should not use stabilizing polynomials with zero as a root. In [1,33] this is enforced by using linear factors of type $\mathbf{I} - \omega_j\mathbf{A}$ in place of $\mu_j\mathbf{I} - \mathbf{A}$ in Theorem 1. All these linear factors, and thus their products, have the value one at zero, i.e., are residual polynomials; similarly, in [13] the Γ-polynomials are constructed such that they are residual polynomials, see (44). In [1] the value of ω_j is chosen to minimize a residual, which might result in a small value of ω_j and thus a large root and thus Ritz value $1/\omega_j$ of the Sonneveld pencil. In [13,33] this scheme is modified using the technique originally presented in [38]; this modification effectively circumvents large roots. The minimization of the norm of the next vector as a function of μ_j is partially justified, as the OR residuals are parallel to the basis vectors; with the technique in [38] this seems to be mostly stable. Other choices we tested are based on the following ideas and combinations thereof:

- We can enforce additional orthogonality, i.e., the first $\mathbf{g}$-vector in a block can be chosen such that it is orthogonal to the last of the previous block.
- We can use approximations to eigenvalues, this is suggested in [9] based on Arnoldi's method and in [10] based on IDR itself. We tried, e.g., the Rayleigh quotient of the last $\mathbf{g}$-vector in the last block.
- We can dampen part of spectrum or the pseudospectrum. Based on estimates on the location of the spectrum or pseudospectrum, we could use, e.g., roots of Faber polynomials or Chebyshev points.
- We can optimize the roots to obtain well-conditioned Hessenberg and upper triangular matrices, or to be as close as possible to the coefficients of the underlying Lanczos$(s, 1)$ process. The latter was a motivation of the modification technique in [38].

We remark that in IDRStab the polynomials are determined at a later stage in the algorithm, where we have gathered some more information, which gives us more possibilities in the optimization of the polynomials, also in the case of degree one. Instead of a GMRes polynomial we tried an ideal GMRes polynomial, i.e., minimized $\|\mathbf{G}_{1,1}^{(k+1)}\|$, see (44). All these ideas have been implemented and are quite successful; yet there are always matrices where one technique is better than the others, no automated best choice of a polynomial has been developed thus far.

5.4. The shadow space

The shadow vectors define the left block Krylov subspace and thus the projection (17). Inserting *a priori* information, i.e., motivated by properties of the system and/or the algorithmic variant, seems to be non-trivial, thus we always use orthonormalized random vectors. In [14] the difference between the resulting "random Galërkin projection" and the minimum residual projection is investigated. On average: the larger s, the closer IDR seems to be to GMRes, at the expense of increased storage and work.

6. Conclusions and outlook

The concept of a generalized Hessenberg decomposition defined in [10] enables us to transfer techniques known for classical Krylov subspace methods to the IDR based methods. To give the answer to the question raised in the title: IDR is an old idea, but the developments that started with IDR(s) are new, even if they are not unexpected given the similarities to classical Krylov subspace methods. Currently, we seek the best IDR variant to compute a stable basis. This IDR variant can than be used to develop a genuine IDR eigenvalue solver and a QMRIDR variant based on stabilizing polynomials of degree larger than one. This is work in progress.

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