A GENERAL FRAMEWORK FOR RECURSIONS FOR KRYLOV SPACE SOLVERS

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Abstract. Krylov space methods for solving linear systems of equations come in many flavors and use various types of recursions to generate iterates x_n (approximate solutions of $Ax = b$), corresponding residuals $r_n := b - Ax_n$, and direction vectors (or search directions) $v_n := (x_{n+1} - x_n)/\omega_n$. Starting from a general definition for a Krylov space solver we give necessary and sufficient conditions for the existence of various types of recursions, and we recall the relations that exist between the matrix representations of these recursions. Much of this is more or less well known, but there are also some new, perhaps even surprising aspects. In particular, we introduce what we call the general inconsistent OrthoRes algorithm, which in contrast to the other recursions is also applicable in situations where for some n the iterate $\mathbf{x}_n$ is not defined due to a so-called pivot breakdown.

1. Introduction. Nowadays, when we refer to iterative methods for solving large sparse linear systems we normally mean Krylov (sub)space solvers. Classical methods that do not belong to this class, like the successive overrelaxation (SOR) method, are no longer competitive, though the matrix splittings of some of them, e.g. the one of SSOR (the symmetric version of SOR), are still used for preconditioning. Multigrid is also an iterative method, but often it is also considered as a preconditioner now. In the past, Krylov space solvers were referred to by different names, in particular semi-iterative methods (Varga, 1962; Young, 1971) and polynomial acceleration methods. Some of them can also be used as preconditioners, in which case they get referred to as polynomial preconditioners. Flexible preconditioning even allows to apply any Krylov space solver as a preconditioner of a Krylov space solver. In this case one often refers to this as an inner-outer iteration method.

Although Krylov (sub)space methods are ubiquitous in scientific computing and several textbooks are nearly exclusively devoted to them, we hardly ever find a mathematical definition of this class. The notion of a Krylov (sub)space is, of course, uniquely defined, and Krylov space solvers are methods based on using such a Krylov space for approximating the solution of a linear system (or, in another application, the eigenvectors of a matrix). There is a large number of specific methods that distinctly belong to this class.

In this paper we actually give a mathematical definition of a Krylov space solver, which, however, contains the vague expression "for most n", and which, moreover, is not general enough to cover all methods that most people would include in the class. In the last section of the paper, we will then extend the definition to cover further well-known examples.

Recurrences for iterates and residuals are a key ingredient of Krylov space solvers. Starting from our definition we derive several well-known types of recurrences, whose existence is seen to hinge on very basic properties of the methods. In this way we will build up a general framework for a large subset of the class of Krylov space solvers. The emphasis is on the properties that allow or disallow a certain type of recurrence and on the connections between these properties, but not on the derivation of specific methods that perform particularly well. So the paper is intended to be a contribution

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to the mathematical basis of Krylov space solvers. In the literature there are other papers with a similar aim, like those of Young and Jea (1980), Jea and Young (1983), Ashby, Manteuffel and Saylor (1990), Ashby and Gutknecht (1993), Weiss (1994*a*), Weiss (1994*b*), Weiss (1996), and Gutknecht and Rozložník (2002). Many of the basic results we present here are well known and are just recalled to make the paper self-contained. Other may be known but difficult to find.

There are Krylov space solvers like GMRES, MINRES, SYMMLQ, and QMR that primarily build up a basis of the Krylov space (or rather of a sequence of spaces) and then solve the linear system approximately in coordinate space. These methods are not covered by our framework yet, but there is the possibility to extend our approach to methods of this type.

2. Krylov Subspaces and Krylov Space Solvers.

We start with a formal definition of a Krylov (sub)space and with various characterizations of its maximum extension.

DEFINITION. Given a nonsingular $N \times N$ matrix $\mathbf{A}$ and an N-vector $\mathbf{y} \neq \mathbf{o}$, the nth **Krylov (sub)space** $\mathcal{K}_n(\mathbf{A}, \mathbf{y})$ generated by $\mathbf{A}$ from $\mathbf{y}$ is

$$\boxed{\mathcal{K}_n :\equiv \mathcal{K}_n(\mathbf{A}, \mathbf{y}) :\equiv \mathsf{span}\,(\mathbf{y}, \mathbf{A}\mathbf{y}, \ldots, \mathbf{A}^{n-1}\mathbf{y}).} \tag{2.1}$$

▲

Clearly, by this definition, whenever $\mathbf{z} \in \mathcal{K}_n(\mathbf{A}, \mathbf{y})$, there is a polynomial p of degree at most $n-1$ such that $\mathbf{z} = p(\mathbf{A})\mathbf{y}$. In general, this polynomial may be not unique since the spanning set in (2.1) may be linearly dependent. We can say more about this case in a moment.

Definition (2.1) associates with a matrix $\mathbf{A}$ and a starting vector $\mathbf{y}$ a whole nested sequence of Krylov subspaces:

$$\mathcal{K}_1 \subseteq \mathcal{K}_2 \subseteq \mathcal{K}_3 \subseteq \ldots .$$

The following lemma answers the question of the equality signs.

LEMMA 2.1. *There is a positive integer* $\bar{\nu} :\equiv \bar{\nu}(\mathbf{y}, \mathbf{A})$ *such that*

$$\boxed{\mathsf{dim}\;\; \mathcal{K}_n(\mathbf{A}, \mathbf{y}) = \begin{cases} n & \text{if} \quad n \leq \bar{\nu}\,, \\ \bar{\nu} & \text{if} \quad n \geq \bar{\nu}\,. \end{cases}}$$

The inequalities $1 \leq \bar{\nu} \leq N$ *hold, and* $\bar{\nu} < N$ *is possible if* $N > 1$.

DEFINITION. The positive integer $\bar{\nu} :\equiv \bar{\nu}(\mathbf{y}, \mathbf{A})$ of Lemma 2.1 is called **grade of y with respect to A**. ▲

PROOF of Lemma 2.1. It follows readily that

$$\mathbf{A}^{\bar{\nu}}\mathbf{y} = \mathbf{y}\gamma_0 + \mathbf{A}\mathbf{y}\gamma_1 + \cdots + \mathbf{A}^{\bar{\nu}-1}\mathbf{y}\gamma_{\bar{\nu}-1}\,, \tag{2.2}$$

where $\gamma_0 \neq 0$ due to the minimality of $\bar{\nu}$. Using this relation we can successively express any $\mathbf{A}^n\mathbf{y}$ with $n > \bar{\nu}$ as a linear combination of $\mathbf{y}$, $\mathbf{A}\mathbf{y}$, ..., $\mathbf{A}^{\bar{\nu}-1}\mathbf{y}$, that is, as an element of $\mathcal{K}_{\bar{\nu}}$. □

There are a number of further characterizations of the index $\bar{\nu}$ of the maximum Krylov subspace $\mathcal{K}_{\bar{\nu}}$. Let us state three of them without proof. Their verification is easy.

Corollary 2.2. *The grade* $\bar{\nu}(\mathbf{y},\mathbf{A})$ *satisfies*

$$\boxed{\begin{aligned}\bar{\nu}(\mathbf{y},\mathbf{A}) &= \min\left\{n \;\middle|\; \dim\ \mathcal{K}_n(\mathbf{A},\mathbf{y}) = \dim\ \mathcal{K}_{n+1}(\mathbf{A},\mathbf{y})\right\} \\ &= \min\left\{n \;\middle|\; \mathcal{K}_n(\mathbf{A},\mathbf{y}) = \mathcal{K}_{n+1}(\mathbf{A},\mathbf{y})\right\}\ .\end{aligned}}$$

Corollary 2.3. *The grade* $\bar{\nu}(\mathbf{y},\mathbf{A})$ *is the dimension of the smallest* $\mathbf{A}$*–invariant subspace that contains* $\mathbf{y}$*.*

Lemma 2.4. *The grade* $\bar{\nu}(\mathbf{y},\mathbf{A})$ *satisfies*

$$\boxed{\bar{\nu}(\mathbf{y},\mathbf{A}) = \min\left\{n \;\middle|\; \mathbf{A}^{-1}\mathbf{y} \in \mathcal{K}_n(\mathbf{A},\mathbf{y})\right\} \le \partial\widehat{\chi}_{\mathbf{A}},}$$

where $\partial\widehat{\chi}_{\mathbf{A}}$ *denotes the degree of the minimal polynomial of* $\mathbf{A}$*.*

For proving here the validity of the $\le$–sign one applies an enhanced form of the Cayley–Hamilton theorem which says that for the minimal polynomial $\widehat{\chi}_{\mathbf{A}}$ of $\mathbf{A}$ holds $\widehat{\chi}_{\mathbf{A}}(\mathbf{A}) = \mathbf{O}$.

From Lemma 2.4 it now follows quickly that once we have constructed a basis of $\mathcal{K}_{\bar{\nu}}(\mathbf{A},\mathbf{r}_0)$ we can find the exact solution of the linear system there.

Corollary 2.5. *Let* $\mathbf{x}_\star$ *be the solution of* $\mathbf{Ax} = \mathbf{b}$ *and let* $\mathbf{x}_0 \ne \mathbf{x}_\star$ *be any initial approximation of it and* $\mathbf{r}_0 :\equiv \mathbf{b} - \mathbf{Ax}_0$ *the corresponding residual. Moreover, let* $\bar{\nu} :\equiv \bar{\nu}(\mathbf{r}_0,\mathbf{A})$*. Then*

$$\boxed{\mathbf{x}_\star \in \mathbf{x}_0 + \mathcal{K}_{\bar{\nu}}(\mathbf{A},\mathbf{r}_0)\,.}$$

Proof. In view of $\mathbf{A}^{-1}\mathbf{r}_0 = \mathbf{A}^{-1}(\mathbf{b} - \mathbf{Ax}_0) = \mathbf{x}_\star - \mathbf{x}_0$ and by Lemma 2.4,

$$\mathbf{x}_\star - \mathbf{x}_0 = -\mathbf{A}^{-1}\mathbf{r}_0 \in \mathcal{K}_{\bar{\nu}}(\mathbf{A},\mathbf{r}_0)\,.$$

□

This corollary shows that if we choose $\mathbf{x}_n$ from the affine space $\mathbf{x}_0 + \mathcal{K}_n(\mathbf{A},\mathbf{r}_0)$ there is a chance that we find the exact solution within (exactly) $\bar{\nu}$ steps. We say then that our method has the **finite termination property**. It is easy to deduce methods that have this property. In fact, it suffices to insure that the residuals $\mathbf{r}_n$ are linearly independent as long as they are nonzero. Of course, once $\mathbf{r}_n = \mathbf{o}$ for some n, the linear system is solved.

However, in practice the finite termination property is nearly irrelevant, since $\bar{\nu}$ is normally much larger than the maximum number of iterations we are willing to execute. We rather want an approximation with sufficiently small residual quickly.

The corollary motivates the following definition.

Definition. A **(standard) Krylov space method for solving a linear system** $\mathbf{Ax} = \mathbf{b}$ or, briefly, a **(standard) Krylov space solver** is an iterative method starting from some initial approximation $\mathbf{x}_0 \ne \mathbf{x}_\star$ and the corresponding residual $\mathbf{r}_0 :\equiv \mathbf{b} - \mathbf{Ax}_0$ and generating for all, or at least most n, iterates $\mathbf{x}_n$ such that

$$\boxed{\mathbf{x}_n - \mathbf{x}_0 = q_{n-1}(\mathbf{A})\mathbf{r}_0 \in \mathcal{K}_n(\mathbf{A},\mathbf{r}_0)} \tag{2.3}$$

with a polynomial q_{n-1} of exact degree $n-1$. ▲

We first note that (2.3) implies that for the error vectors $\mathbf{d}_n :\equiv \mathbf{x}_n - \mathbf{x}_\star$ and for the residual vectors $\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{Ax}_n$ holds

$$\mathbf{d}_n - \mathbf{d}_0 = q_{n-1}(\mathbf{A})\mathbf{r}_0 \in \mathcal{K}_n(\mathbf{A},\mathbf{r}_0)\,, \tag{2.4}$$

$$\mathbf{r}_n - \mathbf{r}_0 = -\mathbf{A}q_{n-1}(\mathbf{A})\mathbf{r}_0 \in \mathbf{A}\mathcal{K}_n(\mathbf{A},\mathbf{r}_0)\,. \tag{2.5}$$

The last relation yields yet another lemma.

LEMMA 2.6. *The residuals of a Krylov space solver satisfy*

$$\boxed{\mathbf{r}_n = p_n(\mathbf{A})\mathbf{r}_0 \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0) \subseteq \mathcal{K}_{n+1}(\mathbf{A}, \mathbf{r}_0)\,,} \tag{2.6}$$

where p_n is a polynomial of degree n, which is related to the polynomial q_{n-1} of (2.3) *by*

$$\boxed{p_n(\zeta) = 1 - \zeta q_{n-1}(\zeta)\,.} \tag{2.7}$$

In particular,

$$\boxed{p_n(0) = 1\,.} \tag{2.8}$$

DEFINITION. The polynomials $p_n \in \mathcal{P}_n$ in (2.6) are the **residual polynomials** of the Krylov space solver. We refer to the condition (2.8) as the **consistency condition** for these polynomials. ▲

As we will see, for some Krylov space solvers there may exist exceptional situations, where for some n the iterate $\mathbf{x}_n$ and the residual $\mathbf{r}_n$ are not defined. It may also occur that the iterates stagnate, so that $\mathbf{x}_{n+1} = \mathbf{x}_n$, which contradicts our assumption that q_n has exact degree n.

Finally, there are **nonstandard Krylov space methods** where the approximation space for $\mathbf{x}_n - \mathbf{x}_0$ is still a Krylov space, but one that differs from $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$. We will treat this case in Section 7.

3. Recursions for Generating a Krylov Space Basis.

By definition of the Krylov space $\mathcal{K}_n(\mathbf{A}, \mathbf{y})$ and by Lemma 2.1 the vectors $\mathbf{y}$, $\mathbf{A}\mathbf{y}$, ..., $\mathbf{A}^{n-1}\mathbf{y}$ form a basis of $\mathcal{K}_n(\mathbf{A}, \mathbf{y})$ as long as $n \le \bar{\nu}(\mathbf{y}, \mathbf{A})$. It is well known that this so-called **Krylov basis** is typically very ill-conditioned as, for $k \to \infty$, the normalized vectors $\mathbf{A}^k\mathbf{y}/\|\mathbf{A}^k\mathbf{y}\|$ converge to an eigenvector associated with the eigenvalue of largest absolute value if there is a single such eigenvalue.

To construct a better basis, we could apply Gram-Schmidt orthogonalization to the Krylov basis. But as suggested by Lanczos (1950) and Arnoldi (1951) it is is far better to combine the Gram-Schmidt process directly with the generation of the basis. Here is a version of the **Arnoldi algorithm** (or **Arnoldi process**) using classical Gram-Schmidt (CGS) orthonormalization.

ALGORITHM 1 (ARNOLDI ALGORITHM BASED ON CGS).
Let a nonsingular matrix $\mathbf{A}$ and a nonzero vector $\mathbf{y}$ be given. For constructing a nested set of orthonormal bases $\{\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_m\}$ for the nested Krylov subspaces $\mathcal{K}_{m+1}(\mathbf{A}, \mathbf{y})$ $(m = 0, \ldots, \bar{\nu}(\mathbf{y}, \mathbf{A}) - 1)$ we let $\eta_0 := \|\mathbf{y}\|$, $\mathbf{y}_0 := \mathbf{y}/\eta_0$ and compute, for $n = 0, 1, \ldots, m-1$,

$$\left.\begin{array}{rcl} \widetilde{\mathbf{y}} & := & (\mathbf{A}\mathbf{y}_n - \mathbf{y}_n\,\eta_{n,n} - \cdots - \mathbf{y}_0\,\eta_{0,n}) \\ \mathbf{y}_{n+1} & := & \widetilde{\mathbf{y}}/\eta_{n+1,n}\,, \end{array}\right\} \tag{3.1}$$

where the coefficients $\eta_{0,n}$, $\eta_{1,n}$, ..., $\eta_{n,n}$ are chosen to make $\widetilde{\mathbf{y}}$ orthogonal to $\mathbf{y}_0$, $\mathbf{y}_1$, ..., $\mathbf{y}_n$, and $\eta_{n+1,n}$ is used to normalize $\widetilde{\mathbf{y}}$:

$$\eta_{k,n} :\equiv \langle \mathbf{y}_k, \mathbf{A}\mathbf{y}_n \rangle \quad (k = 0, \ldots, n), \qquad \eta_{n+1,n} :\equiv \|\widetilde{\mathbf{y}}\|\,. \tag{3.2}$$

When $n = m - 1 = \bar{\nu} - 1$, then $\widetilde{\mathbf{y}} = \mathbf{o}$ and the process terminates.

In practice, in finite precision arithmetic it is much better to integrate the mathematically equivalent modified Gram-Schmidt (MGS) algorithm, but for theoretical work the CGS recursion (3.1)–(3.2) is all we need. The orthonormal basis $\{\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{m-1}\}$ of $\mathcal{K}_m$ $(m \leq \bar{\nu})$ generated here is called the **Arnoldi basis**.

Clearly, in exact arithmetic, the Arnoldi process will terminate with $\eta_{\bar{\nu},\bar{\nu}-1} = 0$ when $n = m - 1 = \bar{\nu} - 1$ since the dimension of the Krylov space generated from $\mathbf{y}$ is exhausted. We therefore define $\mathbf{y}_{\bar{\nu}} :\equiv \mathbf{o}$. This is useful for theoretical considerations. In practice $\eta_{\bar{\nu},\bar{\nu}-1}$ may be far from small due to roundoff errors, but typically m is limited to values much smaller than $\bar{\nu}$.

A disadvantage of the Arnoldi process is that the whole basis must be stored and that at each step all the vectors that have been generated before must be retrieved. There is an important exception: when the matrix is real symmetric or (complex) Hermitian, the long recursion of (3.1) reduces to a three-term recursion, and the Arnoldi process becomes the **symmetric Lanczos process**:

LEMMA 3.1. *If $\mathbf{A} = \mathbf{A}^\star$, then in* (3.1) *with* (3.2) *we have*

$$\eta_{k,n} = 0\,, \qquad k = 0, 1, \ldots, n-2, \tag{3.3}$$

$$\eta_{n-1,n} = \eta_{n,n-1}\,, \tag{3.4}$$

so that if we let $\beta_{-1}^{\mathrm{L}} :\equiv 0$ and

$$\alpha_n^{\mathrm{L}} :\equiv \eta_{n,n} = \langle \mathbf{y}_n, \mathbf{A}\mathbf{y}_n \rangle\,, \tag{3.5a}$$

$$\beta_n^{\mathrm{L}} :\equiv \eta_{n+1,n} = \| \mathbf{A}\mathbf{y}_n - \mathbf{y}_n\, \alpha_n^{\mathrm{L}} - \mathbf{y}_{n-1}\, \beta_{n-1}^{\mathrm{L}} \|\,, \tag{3.5b}$$

the recursion (3.1) *reduces to*

$$\mathbf{y}_{n+1} := \left(\mathbf{A}\mathbf{y}_n - \mathbf{y}_n\, \alpha_n^{\mathrm{L}} - \mathbf{y}_{n-1}\, \beta_{n-1}^{\mathrm{L}} \right) / \beta_n^{\mathrm{L}}\,, \quad n = 0, 1, \ldots, \bar{\nu} - 2\,, \tag{3.6}$$

with $\alpha_n^{\mathrm{L}} \in \mathbb{R}$ $(n = 0, \ldots, \bar{\nu} - 1)$ and $\beta_n^{\mathrm{L}} > 0$ $(n = 0, \ldots, \bar{\nu} - 2)$.

In this case the basis is called **Lanczos basis**, and the vectors $\mathbf{y}_n$ are referred to as **Lanczos vectors**.

PROOF. By construction we have $\mathbf{y}_n \perp \mathbf{y}_i$ for $i = 0, 1, \ldots, n-1$ and $\|\mathbf{y}_j\| = 1$ for $j = 0, 1, \ldots, n$. Therefore, if $k < n - 1$ we can conclude from (3.1) that

$$\begin{aligned} \eta_{k,n} &= \langle \mathbf{y}_k, \mathbf{A}\mathbf{y}_n \rangle = \langle \mathbf{A}\mathbf{y}_k, \mathbf{y}_n \rangle \\ &= \langle \mathbf{y}_{k+1}\eta_{k+1,k} + \mathbf{y}_k\eta_{k,k} + \cdots + \mathbf{y}_0\eta_{0,k}\,,\ \mathbf{y}_n \rangle \\ &= 0\,. \end{aligned}$$

Moreover,

$$\begin{aligned} \alpha_n^{\mathrm{L}} &= \eta_{n,n} = \langle \mathbf{y}_n, \mathbf{A}\mathbf{y}_n \rangle = \langle \mathbf{A}^\star\mathbf{y}_n, \mathbf{y}_n \rangle = \langle \mathbf{A}\mathbf{y}_n, \mathbf{y}_n \rangle = \overline{\langle \mathbf{y}_n, \mathbf{A}\mathbf{y}_n \rangle} = \overline{\alpha_n^{\mathrm{L}}}\,, \\ \beta_n^{\mathrm{L}} &= \eta_{n+1,n} = \| \mathbf{A}\mathbf{y}_n - \mathbf{y}_n\, \alpha_n^{\mathrm{L}} - \mathbf{y}_{n-1}\, \beta_{n-1}^{\mathrm{L}} \| > 0 \end{aligned}$$

except when $n = \bar{\nu} - 1$ where $\beta_{\bar{\nu}-1}^{\mathrm{L}} = 0$. Finally,

$$\begin{aligned} \eta_{n-1,n} &= \langle \mathbf{y}_{n-1}, \mathbf{A}\mathbf{y}_n \rangle = \langle \mathbf{A}\mathbf{y}_{n-1}, \mathbf{y}_n \rangle \\ &= \langle \mathbf{y}_n\eta_{n,n-1} + \mathbf{y}_{n-1}\eta_{n-1,n-1} + \cdots + \mathbf{y}_0\eta_{0,n-1}\,,\ \mathbf{y}_n \rangle \\ &= \langle \mathbf{y}_n, \mathbf{y}_n \rangle\, \overline{\eta_{n,n-1}} \\ &= \eta_{n,n-1}\,. \end{aligned}$$

□

To generate a basis of a Krylov subspace, we can also use recursions of the form (3.1) with other coefficients, because, in view of Lemma 2.1, any such recursion will guarantee that

$$\mathsf{span}\,(\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{n-1}) = \mathsf{span}\,(\mathbf{y}, \mathbf{A}\mathbf{y}, \ldots, \mathbf{A}^{n-1}\mathbf{y}) = \mathcal{K}_n(\mathbf{A}, \mathbf{y})\,. \tag{3.7}$$

Of course, the generated basis will no longer be orthonormal. Moreover, for $n > \bar{\nu}$, the spanning set $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{n-1}$ will no longer be a basis.

In the following we will make heavy use of the fact that recursions for generating Krylov space bases and the recursions for residual vectors, search directions and approximate solutions can be cast in terms of matrix relations. Here we first define the $N \times m$ matrix

$$\mathbf{Y}_m :\equiv \begin{pmatrix} \mathbf{y}_0 & \mathbf{y}_1 & \cdots & \mathbf{y}_{m-1} \end{pmatrix} \tag{3.8}$$

and gather the coefficients of m steps of the recursion (3.1) in an **extended** Hessenberg matrix of size $(m+1) \times m$:

$$\underline{\mathbf{H}}_m :\equiv \begin{pmatrix} \eta_{0,0} & \eta_{0,1} & \cdots & \eta_{0,m-1} \\ \eta_{1,0} & \eta_{1,1} & \cdots & \eta_{1,m-1} \\ & \eta_{2,1} & \ddots & \vdots \\ & & \ddots & \eta_{m-1,m-1} \\ & & & \eta_{m,m-1} \end{pmatrix}. \tag{3.9}$$

Then we can summarize the recursions (3.1) for $n = 0, \ldots, m-1$ as

$$\boxed{\mathbf{A}\mathbf{Y}_m = \mathbf{Y}_{m+1}\underline{\mathbf{H}}_m\,.} \tag{3.10}$$

This is often referred to as **Arnoldi relation**. In the Arnoldi process, the matrices $\mathbf{Y}_m$ have orthonormal columns, but this has not been used in the derivation of (3.10).

$\underline{\mathbf{H}}_m$ can be partitioned into

$$\underline{\mathbf{H}}_m \equiv: \left(\begin{array}{c} \mathbf{H}_m \\ \hline \eta_{m,m-1}\mathbf{l}_m^{\mathsf{T}} \end{array}\right), \tag{3.11}$$

where $\mathbf{l}_m^{\mathsf{T}}$ is the last row of the $m \times m$ unit matrix $\mathbf{I}_m$ and $\mathbf{H}_m$ is square. In the symmetric Lanczos process the matrix $\underline{\mathbf{H}}_m$ reduces to the real **extended** tridiagonal matrix

$$\underline{\mathbf{T}}_m :\equiv \left(\begin{array}{c} \mathbf{T}_m \\ \hline \beta_{m-1}^{\mathrm{L}}\mathbf{l}_m^{\mathsf{T}} \end{array}\right) :\equiv \begin{pmatrix} \alpha_0^{\mathrm{L}} & \beta_0^{\mathrm{L}} & & \\ \beta_0^{\mathrm{L}} & \alpha_1^{\mathrm{L}} & \ddots & \\ & \beta_1^{\mathrm{L}} & \ddots & \beta_{m-2}^{\mathrm{L}} \\ & & \ddots & \alpha_{m-1}^{\mathrm{L}} \\ & & & \beta_{m-1}^{\mathrm{L}} \end{pmatrix}, \tag{3.12}$$

whose square part $\mathbf{T}_m$ is real symmetric — even if $\mathbf{A}$ is (complex) Hermitian.

By (3.10), the image of the restriction $\mathbf{A}\big|_{\mathcal{K}_m}$ to the subspace $\mathcal{K}_m$ of the linear mapping (or, operator) defined by $\mathbf{A}$ is contained in $\mathcal{K}_{m+1}$. With respect to the bases $\mathbf{y}_0, \ldots, \mathbf{y}_{m-1}$ and $\mathbf{y}_0, \ldots, \mathbf{y}_m$ in the domain and the range, respectively, this restricted linear mapping is represented by the $(m+1) \times m$ matrix $\underline{\mathbf{H}}_m$. Let $\mathbf{\Pi}_m$ denote the projection of $\mathcal{K}_{m+1}$ onto $\mathcal{K}_m$ along $\mathbf{y}_m$. If the bases are orthogonal, then so is this projection, but we need not assume this. With $\mathbf{\Pi}_m$ we can project the image $\mathbf{A}\big|_{\mathcal{K}_m}(\mathcal{K}_m)$ into $\mathcal{K}_m$ In terms of the aforementioned bases, $\mathbf{\Pi}_m$ has the simple representation $\left(\begin{array}{c|c} \mathbf{I}_m & \mathbf{o} \end{array}\right)$, and the self-mapping of $\mathcal{K}_m$ defined by $\mathbf{\Pi}\,\mathbf{A}\big|_{\mathcal{K}_m}$ is just

$$\left(\begin{array}{c|c} \mathbf{I}_m & \mathbf{o} \end{array}\right)\underline{\mathbf{H}}_m = \mathbf{H}_m \qquad \text{or} \qquad \left(\begin{array}{c|c} \mathbf{I}_m & \mathbf{o} \end{array}\right)\underline{\mathbf{T}}_m = \mathbf{T}_m\,, \tag{3.13}$$

respectively. The square matrices $\mathbf{H}_m$ and $\mathbf{T}_m$ are therefore often referred to as orthogonal projections of $\mathbf{A}$ into $\mathcal{K}_m$ when the basis is orthonormal.

Once the Krylov space is exhausted, that is, once $m+1 = \bar{\nu}$ and $\eta_{\bar{\nu},\bar{\nu}-1} = 0$, $\mathbf{y}_{\bar{\nu}} = \mathbf{o}$ by definition, and thus the identities (3.10) simplify to

$$\boxed{\mathbf{A}\mathbf{Y}_{\bar{\nu}} = \mathbf{Y}_{\bar{\nu}}\mathbf{H}_{\bar{\nu}}} \qquad \text{and} \qquad \boxed{\mathbf{A}\mathbf{Y}_{\bar{\nu}} = \mathbf{Y}_{\bar{\nu}}\mathbf{T}_{\bar{\nu}}\,.} \tag{3.14}$$

This means that the columns of $\mathbf{Y}_{\bar{\nu}}$ span the invariant subspace $\mathcal{K}_{\bar{\nu}}$ of $\mathbf{A}$. Every eigenvalue of $\mathbf{H}_{\bar{\nu}}$ is also an eigenvalue of $\mathbf{A}$ (but, in general, not vice-versa).

If $\eta_{m,m-1}$ is small, one can expect that the spectrum of $\mathbf{H}_m$ or $\mathbf{T}_m$ approximates in some sense the one of $\mathbf{A}$, although $\mathbf{A}$ has many more eigenvalues than $\mathbf{H}_m$ or $\mathbf{T}_m$ if $N \gg m$. In the Hermitian case this connection is fully explored by the Rayleigh–Ritz procedure and a number of related error bounds; see Parlett (1980). In the case of non-Hermitian matrices the connection between the size of $\eta_{m,m-1}$ and the accuracy of the approximate eigenvalues is more complicated.

Let us next consider the relation between the Arnoldi bases, denoted by $\{\mathbf{y}_n\}_{n=0}^{m-1}$, and some other nested Krylov space bases denoted $\{\widehat{\mathbf{y}}_n\}_{n=0}^{m-1}$, which may be neither normalized nor orthogonal. When we express the new bases in the old ones, then, since the Krylov subspaces and their bases are nested, we have relations of the form

$$\widehat{\mathbf{y}}_k = \mathbf{y}_0\sigma_{0,k} + \mathbf{y}_1\sigma_{1,k} + \cdots + \mathbf{y}_k\sigma_{k,k}\,, \qquad k = 0,\ldots,m.$$

Therefore, the transformation matrix $\mathbf{S}_{m+1} = \left(\begin{array}{c} \sigma_{n,k} \end{array}\right)_{k=0}^{m}$, for which $\widehat{\mathbf{Y}}_{m+1} = \mathbf{Y}_{m+1}\mathbf{S}_{m+1}$ holds, is upper triangular. Thus, $\mathbf{S}_m$ with $\widehat{\mathbf{Y}}_m = \mathbf{Y}_m\mathbf{S}_m$ is just the $m \times m$ leading principal minor of $\mathbf{S}_{m+1}$. So, we have a nested sequence of triangular transformation matrices. When the restricted linear mapping $\mathbf{A}\big|_{\mathcal{K}_m} : \mathcal{K}_m \to \mathcal{K}_{m+1}$ is in the new basis represented by $\widehat{\underline{\mathbf{H}}}_m$, then

$$\boxed{\widehat{\underline{\mathbf{H}}}_m = \mathbf{S}_{m+1}^{-1}\underline{\mathbf{H}}_m\mathbf{S}_m\,.} \tag{3.15}$$

In fact, if $\mathbf{w} = \mathbf{Y}_m\mathbf{k} = \widehat{\mathbf{Y}}_m\widehat{\mathbf{k}}$ and $\mathbf{A}\mathbf{w} = \mathbf{Y}_{m+1}\mathbf{j} = \widehat{\mathbf{Y}}_{m+1}\widehat{\mathbf{j}}$ with $\mathbf{k} = \mathbf{S}_m\widehat{\mathbf{k}}$, $\mathbf{j} = \mathbf{S}_{m+1}\widehat{\mathbf{j}}$, $\mathbf{j} = \underline{\mathbf{H}}_m\mathbf{k}$, and $\widehat{\mathbf{j}} = \widehat{\underline{\mathbf{H}}}_m\widehat{\mathbf{k}}$, then it follows that

$$\widehat{\mathbf{j}} = \mathbf{S}_{m+1}^{-1}\mathbf{j} = \mathbf{S}_{m+1}^{-1}\underline{\mathbf{H}}_m\mathbf{k} = \mathbf{S}_{m+1}^{-1}\underline{\mathbf{H}}_m\mathbf{S}_m\widehat{\mathbf{k}} = \widehat{\underline{\mathbf{H}}}_m\widehat{\mathbf{k}}$$

if $\widehat{\underline{\mathbf{H}}}_m$ satisfies (3.15). So, the following holds:

LEMMA 3.2. *Any generation of a nested sequence of bases for a nested sequence of Krylov subspaces can be represented by a matrix identity of the form* (3.10) *with a nested sequence of extended upper Hessenberg matrices* $\underline{\mathbf{H}}_m$ $(m = 1,\ldots,\bar{\nu})$ *with nonzero elements on the first subdiagonal, except for* $\eta_{\bar{\nu},\bar{\nu}-1} = 0$ *if* $m+1 = \bar{\nu}$.

A basis transformation in such a nested sequence of Krylov subspaces is expressed by a nested sequence of upper triangular matrices $\mathbf{S}_m$ $(m = 1, 2, \ldots)$. *The two sets of Hessenberg matrices describing the generation of the two sets of bases are then related by* (3.15).

A particularly simple special case is when we rescale a basis, that is, just change the length of the basis vectors. In this case, the matrices $\mathbf{S}_m$ are nested diagonal matrices.

Actually, the value $\eta_{\bar{\nu},\bar{\nu}-1} = 0$ is irrelevant for the compact representation of the recursion (3.1) since $\widetilde{\mathbf{y}} = \mathbf{o}$ in this case: $\mathbf{Y}_{\bar{\nu}+1}\underline{\mathbf{H}}_{\bar{\nu}} = \mathbf{Y}_{\bar{\nu}}\mathbf{H}_{\bar{\nu}}$ does not depend on $\eta_{\bar{\nu},\bar{\nu}-1}$. But from the theoretical point of view it is important that the Arnoldi algorithm discovers that $\mathbf{A}\mathbf{y}_{\bar{\nu}-1} \in \mathcal{K}$, that is, that the Krylov space is exhausted: this property will allow us to implement methods that have the finite termination property.

In this connection we mention that the recursion (3.1) may also be used for generating a sequence of vectors that has more than $\bar{\nu}$ elements. Then, for $n \geq \bar{\nu}$ these vectors will no longer be linearly independent. But also in this case, where $\eta_{\bar{\nu},\bar{\nu}-1} \neq 0$, the matrix identity (3.10) remains valid. An example is Chebyshev iteration.

4. Recursions for Iterates and Residuals. In this section, we start from our general definition of a standard Krylov space solver in Section 2 and derive recursions for the iterates and residuals of any such solver. In the last section we have only considered the generation of Krylov space bases, but not yet the solution of a linear system. However, the recursion (3.1) for generating a basis is easily turned into recursions for generating iterates $\mathbf{x}_n$ and corresponding residuals $\mathbf{r}_n$. For brevity, also these residuals and iterates are gathered into matrices

$$\mathbf{R}_m :\equiv \begin{pmatrix} \mathbf{r}_0 & \mathbf{r}_1 & \cdots & \mathbf{r}_{m-1} \end{pmatrix}, \quad \mathbf{X}_m :\equiv \begin{pmatrix} \mathbf{x}_0 & \mathbf{x}_1 & \cdots & \mathbf{x}_{m-1} \end{pmatrix}.$$

We first assume that the residuals and iterates generated for a particular example exist for all n up to m and are known. We claim that they always satisfy a certain type of recursion formula.

THEOREM 4.1. *If defined for all n up to m, the iterates $\mathbf{x}_n$ and the residuals $\mathbf{r}_n$ of a Krylov space solver satisfy, for $n = 0, 1, \ldots, m-1$, recursions of the form*

$$\boxed{\mathbf{r}_{n+1} := \left(\mathbf{A}\mathbf{r}_n - \mathbf{r}_n\,\eta^\circ_{n,n} - \cdots - \mathbf{r}_0\,\eta^\circ_{0,n}\right)/\eta^\circ_{n+1,n}\,,} \tag{4.1}$$

$$\boxed{\mathbf{x}_{n+1} := -\left(\mathbf{r}_n + \mathbf{x}_n\,\eta^\circ_{n,n} + \cdots + \mathbf{x}_0\,\eta^\circ_{0,n}\right)/\eta^\circ_{n+1,n}} \tag{4.2}$$

with

$$\boxed{\eta^\circ_{n+1,n} :\equiv -\,\eta^\circ_{n,n} - \eta^\circ_{n-1,n} - \cdots - \eta^\circ_{0,n}\,.} \tag{4.3}$$

Equivalently,

$$\boxed{\mathbf{R}_m = -\mathbf{X}_{m+1}\underline{\mathbf{H}}^\circ_m\,, \qquad \mathbf{A}\mathbf{R}_m = \mathbf{R}_{m+1}\underline{\mathbf{H}}^\circ_m\,,} \tag{4.4}$$

where $\underline{\mathbf{H}}^\circ_m :\equiv (\eta^\circ_{k,l})$ is an $(m+1)\times m$ extended Hessenberg matrix with column sums 0 whose leading principal submatrices are all nonsingular.

PROOF. By definition (2.3), for any Krylov space solver, one has $\mathbf{x}_n - \mathbf{x}_0 = q_{n-1}(\mathbf{A})\mathbf{r}_0 \in \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ with a polynomial q_{n-1} of exact degree $n-1$, and by Lemma 2.6 the nth residual satisfies $\mathbf{r}_n = p_n(\mathbf{A})\mathbf{r}_0$, where q_{n-1} and the nth residual polynomial p_n, which has exact degree n, are related by $p_n(\zeta) = 1 - \zeta\, q_{n-1}(\zeta)$, see (2.7). So, the vectors $\mathbf{r}_0, \ldots, \mathbf{r}_{n-1}$ span $\mathcal{K}_n$ (even when they are linearly dependent, in which case $\mathcal{K}_n = \mathcal{K}_{n-1}$). Therefore, if we define the extended $(m+1)\times m$ Frobenius (or companion) matrix

$$\underline{\mathbf{F}}_m := \begin{pmatrix} -1 & -1 & \cdots & -1 \\ 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}, \tag{4.5}$$

then we have, in view of $\mathbf{x}_n - \mathbf{x}_0 \in \mathcal{K}_n$,

$$\mathbf{X}_{m+1}\underline{\mathbf{F}}_m = -\,\mathbf{R}_m\mathbf{U}_m \tag{4.6}$$

with some upper triangular $m\times m$ matrix $\mathbf{U}_m$ and an extra minus sign. Since both $\mathbf{x}_{n+1}$ and $\mathbf{r}_n$ are represented by polynomials of exact degree n, the diagonal elements of $\mathbf{U}_m$ do not vanish (or, if the residuals are linearly dependent, these elements can be chosen not to vanish).

Each column sum in $\underline{\mathbf{F}}_m$ is zero, *i.e.*, $\begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix} \underline{\mathbf{F}}_m = \mathbf{o}^{\mathsf{T}}$, and therefore, for an arbitrary N-vector $\mathbf{b}$, multiplication of $\underline{\mathbf{F}}_m$ from the left by the $N\times(m+1)$ matrix $\begin{pmatrix} \mathbf{b} & \mathbf{b} & \cdots & \mathbf{b} \end{pmatrix}$ yields an $N\times m$ zero matrix. Therefore,

$$\mathbf{R}_{m+1}\underline{\mathbf{F}}_m = \left(\begin{pmatrix} \mathbf{b} & \cdots & \mathbf{b} \end{pmatrix} - \mathbf{A}\mathbf{X}_{m+1}\right)\underline{\mathbf{F}}_m = -\mathbf{A}\mathbf{X}_{m+1}\underline{\mathbf{F}}_m = \mathbf{A}\mathbf{R}_m\mathbf{U}_m\,. \tag{4.7}$$

Hence, if we let

$$\underline{\mathbf{H}}^{\circ}_m :\equiv \underline{\mathbf{F}}_m\mathbf{U}_m^{-1}\,, \tag{4.8}$$

we can write (4.6)–(4.7) as (4.4), where $\underline{\mathbf{H}}^{\circ}_m$ is an $(m+1)\times m$ unreducible upper Hessenberg matrix whose m leading principal submatrices are all nonsingular. In particular, the subdiagonal elements $\eta^{\circ}_{n+1,n}$ are all nonzero. As a consequence of $\mathbf{e}^{\mathsf{T}}\underline{\mathbf{F}}_m = \mathbf{o}^{\mathsf{T}}$, this matrix satisfies

$$\mathbf{e}^{\mathsf{T}}\underline{\mathbf{H}}^{\circ}_m = \mathbf{o}^{\mathsf{T}}, \qquad \text{where} \quad \mathbf{e}^{\mathsf{T}} :\equiv \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix}. \tag{4.9}$$

□

ALGORITHM 2 (ORTHORES FORM OF A KRYLOV SPACE SOLVER).
The ORTHORES *form of a Krylov space method for solving* $\mathbf{A}\mathbf{x} = \mathbf{b}$ *applies the recursions* (4.1)–(4.3)*. They just require an initial approximation* $\mathbf{x}_0$ *and the corresponding residual* $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$*. The coefficients* $\eta^{\circ}_{k,n}$*,* $(k = 0,\ldots,n;\ n = 0,\ldots,m-1)$ *depend on the particular solver;* $\eta^{\circ}_{n+1,n}$ *is given by* (4.3) *and must be nonzero.*

This is a straightforward generalization of the classical ORTHORES method (Young and Jea, 1980), where the residuals are chosen orthogonal (hence the name), and thus the coefficients $\eta^{\circ}_{k,n}$ are for $k \le n$ determined as in the Arnoldi algorithm.

We claim that the property (4.3) of zero column sums is the **matrix version of the consistency condition** for Krylov space solvers. Note that this property is inherited from $\underline{\mathbf{F}}_m$. Recall that we introduced a consistency condition for the residual polynomials p_n, namely $p_n(0) = 1$ from (2.8), which we obtained by inserting $\zeta = 0$ into (2.7). We want to show that the two conditions are equivalent.

We start by casting the recursions of the residual polynomials p_n and those for the polynomials associated to the basis vectors $\mathbf{y}_n$ in terms of the Hessenberg matrices $\underline{\mathbf{H}}^{\circ}_m$ and $\underline{\mathbf{H}}_m$ representing the recursions for the vectors $\mathbf{r}_n$ and $\mathbf{y}_n$, respectively. Denote the latter polynomials by t_n, so that $\mathbf{y}_n = t_n(\mathbf{A})\mathbf{y}_0$. Then (4.1) and (3.1), when translated into polynomial space, become

$$p_{n+1}(\tau) := \left((\tau - \eta^{\circ}_{n,n})p_n(\tau) - \eta^{\circ}_{n-1,n}p_{n-1}(\tau) - \cdots - \eta^{\circ}_{0,n}p_0(\tau)\right)/\eta^{\circ}_{n+1,n}\,, \tag{4.10a}$$

$$t_{n+1}(\tau) := \left((\tau - \eta_{n,n})t_n(\tau) - \eta_{n-1,n}t_{n-1}(\tau) - \cdots - \eta_{0,n}t_0(\tau)\right)/\eta_{n+1,n}\,, \tag{4.10b}$$

with $p_0(\tau) :\equiv 1$, $t_0(\tau) :\equiv 1$. If we let

$$\mathbf{p}_m^{\mathsf{T}} :\equiv \left(\begin{array}{cccc} p_0 & p_1 & \cdots & p_{m-1} \end{array} \right), \qquad \mathbf{t}_m^{\mathsf{T}} :\equiv \left(\begin{array}{cccc} t_0 & t_1 & \cdots & t_{m-1} \end{array} \right), \tag{4.11}$$

then, for $n = 0, \ldots, m-1$, these recursions can be summarized as

$$\boxed{\tau\, \mathbf{p}_m^{\mathsf{T}}(\tau) = \mathbf{p}_{m+1}^{\mathsf{T}}(\tau)\, \underline{\mathbf{H}}_m^{\circ}\,, \qquad \tau\, \mathbf{t}_m^{\mathsf{T}}(\tau) = \mathbf{t}_{m+1}^{\mathsf{T}}(\tau)\, \underline{\mathbf{H}}_m\,.} \tag{4.12}$$

From the first one we see that $p_n(0) = 1$ $(n = 0, \ldots, m)$ is equivalent to $\mathbf{e}^{\mathsf{T}} \underline{\mathbf{H}}_m^{\circ} = \mathbf{o}^{\mathsf{T}}$ from (4.9). The second one yields

$$\boxed{\mathbf{t}_{m+1}^{\mathsf{T}}(0)\, \underline{\mathbf{H}}_m = \mathbf{o}^{\mathsf{T}}\,,} \tag{4.13}$$

which is shorthand for a recursion obtained from (4.10b) for computing $t_n(0)$ recursively:

$$t_{n+1}(0) := -\left(\eta_{n,n} t_n(0) - \eta_{n-1,n} t_{n-1}(0) - \cdots - \eta_{0,n} t_0(0)\right) / \eta_{n+1,n}\,. \tag{4.14}$$

Here is a formal statement of the equivalence result just shown:

THEOREM 4.2. *The consistency condition $p_n(0) = 1$ for the residual polynomials and the consistency condition (4.3) (or, (4.9)) for the Hessenberg matrices containing the recurrence coefficients are equivalent.*

Next we want to explore further the relationship between the Arnoldi-like recursion (3.1) and the residual recursion (4.1) in OrthoRes. We assume an arbitrary choice of $\eta_{k,n}$ $(k = 0, \ldots, n)$ in (4.1). Given $\{\mathbf{y}_n\}_{n=0}^m$ generated by (3.1), we can rescale this sequence by dividing $\mathbf{y}_n$ by $t_n(0)$, so that $\mathbf{r}_n :\equiv \mathbf{y}_n / t_n(0)$ becomes a sequence of residuals, since the associated polynomials $p_n(\tau) :\equiv t_n(\tau)/t_n(0)$ are then normalized at $\tau = 0$. Clearly, this is possible if and only if $t_n(0) \neq 0$ $(\forall n)$. In the matrix formulation, this scaling amounts to multiplying $\mathbf{t}_m^{\mathsf{T}}$ by $\mathbf{D}_{t;m}^{-1}$, where

$$\mathbf{D}_{t;m} :\equiv \mathsf{diag}\ (t_0(0), \ldots, t_{m-1}(0))\ . \tag{4.15}$$

Hence, the two identities in (4.12) are related as follows:

$$\tau\, \underbrace{\mathbf{t}_m^{\mathsf{T}}(\tau) \mathbf{D}_{t;m}^{-1}}_{\mathbf{p}_m^{\mathsf{T}}(\tau)} = \underbrace{\mathbf{t}_{m+1}^{\mathsf{T}}(\tau) \mathbf{D}_{t;m+1}^{-1}}_{\mathbf{p}_{m+1}^{\mathsf{T}}(\tau)} \underbrace{\mathbf{D}_{t;m+1} \underline{\mathbf{H}}_m \mathbf{D}_{t;m}^{-1}}_{\underline{\mathbf{H}}_m^{\circ}}\ . \tag{4.16}$$

That is, by an "extended diagonal similarity transformation" the extended Hessenberg matrix $\underline{\mathbf{H}}_m$ can be scaled to become one with zero column sums, provided $t_n(0) \neq 0$ $(n = 0, \ldots, m)$. This transformation is a special case of (3.15) with $\mathbf{S}_m = \mathbf{D}_{t;m}^{-1}$. The corresponding transformation between the two matrix relations (3.10) and (4.4) is

$$\mathbf{A}\, \underbrace{\mathbf{Y}_m \mathbf{D}_{t;m}^{-1}}_{\mathbf{R}_m} = \underbrace{\mathbf{Y}_{m+1} \mathbf{D}_{t;m+1}^{-1}}_{\mathbf{R}_{m+1}} \underbrace{\mathbf{D}_{t;m+1} \underline{\mathbf{H}}_m \mathbf{D}_{t;m}^{-1}}_{\underline{\mathbf{H}}_m^{\circ}}\ . \tag{4.17}$$

We conclude that the following holds:

THEOREM 4.3. *Given an extended upper $(m+1) \times m$ Hessenberg matrix $\underline{\mathbf{H}}_m = (\eta_{k,l})$ with nonzero subdiagonal elements, let $t_0 :\equiv 1$, let $t_n(0)$, $n = 1, \ldots, m$, be defined by the recursion (4.14), and let $\mathbf{D}_{t;m}$ be given by (4.15). Assume that $t_n(0) \neq 0$, $n = 1, \ldots, m$. Then the transformation $\mathbf{D}_{t;m+1} \mathbf{H}_m \mathbf{D}_{t;m}^{-1}$ turns $\underline{\mathbf{H}}_m$ into an extended Hessenberg matrix $\underline{\mathbf{H}}_m^{\circ}$ with nonzero subdiagonal elements and vanishing column sums.*
If $t_m(0) = 0$ or $\eta_{m,m-1} = 0$, then $\eta_{m,m-1}^{\circ} = 0$.

If we delete the last rows of $\underline{\mathbf{H}}_m$ and $\underline{\mathbf{H}}^\circ_m$ and concentrate on the square matrices $\mathbf{H}_m$ and $\mathbf{H}^\circ_m$, we can reformulate and invert this theorem in the following way.

THEOREM 4.4. *Given an irreducible upper Hessenberg matrix* $\mathbf{H}_m = (\eta_{k,l})_{k,l=0}^{m-1}$, *let* $t_0 :\equiv 1$, *and let* $t_n(0)$, $n = 1, \ldots, m-1$, *be defined by the recursion* (4.14). *Then there is a diagonal similarity transformation* $\mathbf{D}_{t;m}\mathbf{H}_m\mathbf{D}_{t;m}^{-1}$ *that turns* $\mathbf{H}_m$ *into an irreducible Hessenberg matrix* $\mathbf{H}^\circ_m$ *with vanishing column sums in all columns but the last one if and only if* $t_n(0) \neq 0$, $n = 1, \ldots, m-1$. *If the latter holds,* $\mathbf{D}_{t;m}$ *is up to a nonzero scalar factor given by* (4.15).

PROOF. One direction of the claim has been established above: if $t_n(0) \neq 0$, $n = 1, \ldots, m-1$, our construction yields $\mathbf{H}^\circ_m$ with $m-1$ vanishing column sums.

To prove the converse, we try to construct the diagonal similarity transformation with the mentioned properties directly from the condition $\mathbf{D}_{t;m}\mathbf{H}_m\mathbf{D}_{t;m}^{-1} = \mathbf{H}^\circ_m$. The first element, $\delta_0 \neq 0$ of $\mathbf{D}_{t;m}$ can be chosen arbitrarily. To make the first column sum vanish, we need to choose δ_1 so that $\delta_0\, \eta_{0,0} + \delta_1\, \eta_{1,0} = 0$. Likewise, to make the $(n+1)$th column sum zero we have to choose δ_{n+1} such that

$$\delta_0\, \eta_{0,n} + \delta_1\, \eta_{1,n} + \cdots + \delta_n\, \eta_{n,n} + \delta_{n+1}\, \eta_{n+1,n} = 0\,.$$

Hence, $\mathbf{D}_{t;m}$ is uniquely determined if it exists and if it is normalized by $\delta_0 := 1$. Moreover, the above condition translates into the recursion (4.14) if we identify δ_n with $t_n(0)$, and the resulting matrix $\mathbf{D}_{t;m}$ provides a similarity transformation if and only if it is nonsingular. □

The following, well-known result sheds more light on the condition we found.

THEOREM 4.5. *The eigenvalues of the irreducible Hessenberg matrix* $\mathbf{H}_m$ *are the zeros of* t_m, *that is, up to normalization* t_m *is the characteristic polynomial of* $\mathbf{H}_m$. *An analogue statement holds for* $\mathbf{H}^\circ_m$ *and* p_m.

PROOF. One approach to proving this theorem consists in expanding $\chi_{\mathbf{H}_m}(\lambda) :\equiv \det\,(\lambda\mathbf{I} - \mathbf{H}_m)$ along its last column in order to show that the characteristic polynomials $\chi_{\mathbf{H}_n}$ of the leading principal submatrices $\mathbf{H}_n$ satisfy the same recursion as suitably scaled versions of the polynomial t_n. Details are left to the reader.

The fact that every zero of t_m is an eigenvalue of $\mathbf{H}_m$ (and every zero of p_m is an eigenvalue of $\mathbf{H}^\circ_m$) is also seen from (4.12), whose second formula may be written

$$\boxed{\mathbf{t}_m^{\mathsf{T}}(\tau)(\tau\mathbf{I} - \mathbf{H}_m) = t_m(\tau)\eta_{m,m-1}\mathbf{l}_m^{\mathsf{T}}\,.} \tag{4.18}$$

If $t_m(\tau) = 0$, the row vector $\mathbf{t}_m^{\mathsf{T}}(\tau)$ (which is not the zero vector since its first component t_0 is a nonzero constant) is a left eigenvector for the eigenvalue τ. □

Theorem 4.5 has two simple corollaries:

COROLLARY 4.6. *Assume that* $t_n(0) \neq 0$, $n = 1, \ldots, m-1$, *and let* $\mathbf{t}_m^{\mathsf{T}}$, $\mathbf{p}_m^{\mathsf{T}}$, $\mathbf{H}_m$, *and* $\mathbf{H}^\circ_m$ *be related as in* (4.16). *Then the zeros of* t_m *are equal to those of* p_m *and thus equal to the eigenvalues of* $\mathbf{H}^\circ_m$. *Consequently,* p_m *is a scalar multiple of* t_m.

PROOF. The relation $\mathbf{D}_{t;m+1}\underline{\mathbf{H}}_m\mathbf{D}_{t;m}^{-1} = \underline{\mathbf{H}}^\circ_m$ in (4.16) implies that $\mathbf{D}_{t;m}\mathbf{H}_m\mathbf{D}_{t;m}^{-1} = \mathbf{H}^\circ_m$, that is, the matrices $\mathbf{H}_m$ and $\mathbf{H}^\circ_m$ are similar. Also, by Theorem 4.5 the polynomials t_m and p_m are up to normalization the characteristic polynomials of $\mathbf{H}_m$ and $\mathbf{H}^\circ_m$, respectively. □

COROLLARY 4.7. *The following statements are equivalent:*

(i) $t_n(0) \neq 0$, $n = 1, \ldots, m-1$;

(ii) all leading principal submatrices $\mathbf{H}_n$, $n = 1, \ldots, m-1$, *of* $\mathbf{H}_m$ *are nonsingular.*

(iii) $\mathbf{H}_m$ *has a Gaussian LU decomposition (without pivoting) such that* $\mathbf{H}_m = \mathbf{L}_m\mathbf{U}_m$, *where* $\mathbf{U}_m$ *is unit upper triangular and* $\mathbf{L}_m$ *is lower triangular and has at least* $m-1$ *nonzero leading diagonal elements.*

PROOF. (i) $\iff$ (ii): this is an immediate consequence of Theorem 4.5. (ii) $\implies$ (iii) is a well-known fact about Gaussian elimination: in particular, when in Gaussian elimination a pivot becomes zero, then the decomposition can be completed without pivoting only if the reduced system matrix is zero. (The last row of the row-echelon form of the matrix is reached.) Here, this happens if $\mathbf{H}_m$ is singular, in which case the last diagonal element of $\mathbf{L}_m$ is zero. Conversely, since $\mathbf{H}_m = \mathbf{L}_m \mathbf{U}_m$ implies that $\mathbf{H}_n = \mathbf{L}_n \mathbf{U}_n$ $(n = 1, \ldots, m-1)$, the nonsingularity of $\mathbf{L}_n$ and $\mathbf{U}_n$ for $n = 1, \ldots, m-1$ implies the nonsingularity of $\mathbf{H}_n$. $\square$

Recall from what we said at the end of Section 3 that if the Krylov space solver described by $\underline{\mathbf{H}}^\circ_{\bar{\nu}}$ has the finite termination property, then the last column of $\mathbf{H}^\circ_{\bar{\nu}}$ is determined (up to a scalar factor) by the representation of $\mathbf{A}\mathbf{r}_{\bar{\nu}-1}$ in terms of the basis $\mathbf{r}_0, \ldots, \mathbf{r}_{\bar{\nu}-1}$ of $\mathcal{K}_{\bar{\nu}}$:

$$\mathbf{A}\mathbf{r}_{\bar{\nu}-1} = \mathbf{r}_{\bar{\nu}-1}\eta^\circ_{\bar{\nu}-1,\bar{\nu}-1} + \cdots + \mathbf{r}_0\eta^\circ_{0,\bar{\nu}-1}\,.$$

If different coefficients are used in (4.1), then the method will not have the finite termination property.

5. The Inconsistent OrthoRes Algorithm. When the ORTHORES algorithm breaks down for some $n < \bar{\nu} - 1$ due to $\eta^\circ_{n+1,n} = 0$ (which goes along with $t_n(0) = 0$ as is seen from (4.15) and (4.16); cf. Theorem 4.3), this is called a **pivot breakdown**. We can no longer compute $\mathbf{x}_{n+1}$ and $\mathbf{r}_{n+1}$, but we can still compute $\mathbf{y}_{n+1}$ (scaled arbitrarily) and proceed building up this sequence. A corresponding sequence of incorrectly scaled iterates $\widehat{\mathbf{x}}_n$ can also be generated, and, once $t_m(0) \neq 0$ for some $m > n$, we can rescale $\widehat{\mathbf{x}}_m$ and $\mathbf{y}_m$ to find $\mathbf{x}_m$ and $\mathbf{r}_m$. This is what we call the **inconsistent** ORTHORES **form** of a Krylov space solver whose iterates need not exist for all n. A version of the biconjugate gradient (BICG) method based on this idea was first presented in Gutknecht (1990) and Gutknecht (1992) as the "unnormalized" BIORES algorithm; in Gutknecht (1997) it was renamed inconsistent BIORES algorithm. Here are the details of the general inconsistent ORTHORES algorithm:

ALGORITHM 3 (INCONSISTENT ORTHORES FORM OF A KRYLOV SPACE SOLVER). *In the* ORTHORES *form of a Krylov space method for solving* $\mathbf{A}\mathbf{x} = \mathbf{b}$ *we choose an initial approximation* $\mathbf{x}_0$ *and let* $\mathbf{y}_0 := (\mathbf{b} - \mathbf{A}\mathbf{x}_0)/\eta_{-1}$ *with some* $\eta_{-1} \neq 0$. *(For example, we choose* $\eta_{-1} := \|\mathbf{b} - \mathbf{A}\mathbf{x}_0\|$ *or* $\eta_{-1} := 1$.*) Then we let* $\widehat{\mathbf{x}}_0 := \mathbf{x}_0/\eta_{-1}$, $t_0(0) := 1/\eta_{-1}$ *and compute, for* $n = 0, 1, \ldots,$

- $\mathbf{y}_{n+1}$ *according to*

$$\boxed{\mathbf{y}_{n+1} := (\mathbf{A}\mathbf{y}_n - \mathbf{y}_n\,\eta_{n,n} - \cdots - \mathbf{y}_0\,\eta_{0,n})\,/\eta_{n+1,n}} \tag{5.1}$$

  with $\eta_{n+1,n} \neq 0$ *(e.g., such that* $\|\mathbf{y}_{n+1}\| = 1$*),*

- $\widehat{\mathbf{x}}_{n+1}$ *according to*

$$\boxed{\widehat{\mathbf{x}}_{n+1} := -\ (\mathbf{y}_n + \widehat{\mathbf{x}}_n\,\eta_{n,n} + \cdots + \widehat{\mathbf{x}}_0\,\eta_{0,n})\,/\eta_{n+1,n}\,,} \tag{5.2}$$

- $t_{n+1}(0)$ *according to* (4.14), *i.e.,*

$$\boxed{t_{n+1}(0) := -\,(t_n(0)\eta_{n,n} - \cdots - t_0(0)\eta_{0,n})\,/\eta_{n+1,n}\,,} \tag{5.3}$$

- *if* $\|\mathbf{y}_{n+1}\|/|t_{n+1}(0)| < tol$, *set*

$$\boxed{\mathbf{x}_{n+1} := \frac{\widehat{\mathbf{x}}_{n+1}}{t_{n+1}(0)}, \qquad \mathbf{r}_{n+1} := \frac{\mathbf{y}_{n+1}}{t_{n+1}(0)}} \tag{5.4}$$

  and stop.

The coefficients $\eta_{k,n}$, $(k = 0, \ldots, n;\ n = 0, 1, \ldots, m-1)$ *depend on the particular solver;* $\eta_{n+1,n} \neq 0$ *can be chosen freely. Pivot breakdowns do not occur.*

THEOREM 5.1. *In the inconsistent* ORTHORES *algorithm* $\mathbf{y}_n$ *and* $\widehat{\mathbf{x}}_n$ *are related by*

$$\boxed{\mathbf{y}_n = \mathbf{b}t_n(0) - \mathbf{A}\widehat{\mathbf{x}}_n\,.} \tag{5.5}$$

In particular, in (5.4) $\mathbf{r}_{n+1}$ *is the residual of* $\mathbf{x}_{n+1}$, *that is,* $\mathbf{r}_{n+1} = \mathbf{b} - \mathbf{A}\mathbf{x}_{n+1}$. *If* $\mathbf{y}_{n+1}\eta_{n+1,n} = \mathbf{o}$, *then* $n + 1 = \bar{\nu}$, $t_{n+1}(0) \neq 0$, *and* $\mathbf{x}_\star = \mathbf{x}_{n+1} = \widehat{\mathbf{x}}_{n+1}/t_{n+1}(0)$.

PROOF. For $n = 0$, (5.5) is correct. Assume it is correct up to the index n. Then by (5.1)–(5.3))

$$\begin{aligned}
&(\mathbf{b}t_{n+1}(0) - \mathbf{A}\widehat{\mathbf{x}}_{n+1})\eta_{n+1,n} \\
&= -\mathbf{b}\,(t_n(0)\eta_{n,n} + t_{n-1}(0)\eta_{n-1,n} + \cdots + t_0(0)\eta_{0,n}) \\
&\quad + \mathbf{A}\mathbf{y}_n + \mathbf{A}\widehat{\mathbf{x}}_n\eta_{n,n} + \mathbf{A}\widehat{\mathbf{x}}_{n-1}\eta_{n-1,n} + \cdots + \mathbf{A}\widehat{\mathbf{x}}_0\eta_{0,n} \\
&= \mathbf{A}\mathbf{y}_n - \mathbf{y}_n\eta_{n,n} - \mathbf{y}_{n-1}\eta_{n-1,n} - \cdots - \mathbf{y}_0\eta_{0,n} \\
&= \mathbf{y}_{n+1}\eta_{n+1,n}\,.
\end{aligned}$$

So, (5.5) follows by induction. It implies that in (5.4) $\mathbf{r}_{n+1}$ is the residual of $\mathbf{x}_{n+1}$.

When the algorithm terminates due to $\mathbf{y}_{n+1} = \mathbf{o}$, then $n+1 = \bar{\nu}$ and the eigenvalues of $\mathbf{H}_{\bar{\nu}}$ are also eigenvalues of $\mathbf{A}$. Since by Theorem 4.5 the eigenvalues of $\mathbf{H}_{n+1}$ are the zeros of t_{n+1}, it follows from our assumption of a nonsingular $\mathbf{A}$, that $t_{n+1}(0) \neq 0$. So $\mathbf{r}_{n+1} = \mathbf{o}$ and $\mathbf{x}_{n+1} = \mathbf{x}_\star$. □

In terms of recursion coefficient matrices, the recursions (5.1)-(5.3) translate into

$$\boxed{\mathbf{Y}_m = -\widehat{\mathbf{X}}_{m+1}\underline{\mathbf{H}}_m\,, \qquad \mathbf{A}\mathbf{Y}_m = \mathbf{Y}_{m+1}\underline{\mathbf{H}}_m} \tag{5.6}$$

and, in view of $\mathbf{t}_n^{\mathsf{T}}(0) = \mathbf{e}^{\mathsf{T}}\mathbf{D}_{t;n}$,

$$\boxed{\mathbf{t}_{m+1}^{\mathsf{T}}(0)\underline{\mathbf{H}}_m = \mathbf{e}^{\mathsf{T}}\mathbf{D}_{t;m+1}\underline{\mathbf{H}}_m = \mathbf{o}^{\mathsf{T}}\,.} \tag{5.7}$$

Finally, (5.4) becomes

$$\boxed{\widehat{\mathbf{X}}_{m+1} = \mathbf{X}_{m+1}\mathbf{D}_{t;m+1}\,, \qquad \mathbf{Y}_{m+1} = \mathbf{R}_{m+1}\mathbf{D}_{t;m+1}\,.} \tag{5.8}$$

With this notation it is easy to verify that the approximate solutions $\mathbf{x}_n$ found in this way are (in exact arithmetic) identical to those of ORTHORES as long as the latter does not break down.

THEOREM 5.2. *If $t_n \neq 0$ for $n = 0, \ldots, m$, the approximants $\mathbf{x}_{n+1}$ generated according to (5.4) are identical to those generated by the* ORTHORES *algorithm 2 with the coefficient matrix $\underline{\mathbf{H}}^\circ_m := \mathbf{D}_{t;m+1}\underline{\mathbf{H}}_m\mathbf{D}^{-1}_{t;m}$.*

PROOF. Inserting (5.8) into the relations (5.6) leads via (4.17) to the relations (4.4) of ORTHORES. □

From Theorem 5.1 and the connection to the general Arnoldi-like construction of Krylov space bases discussed in Section 3 we can further conclude that the following holds:

THEOREM 5.3. *Given any nonsingular square system $\mathbf{A}\mathbf{x} = \mathbf{b}$ and any initial approximation $\mathbf{x}_0$ and the corresponding residual $\mathbf{r}_0$, a nested set of bases for the nested set of Krylov subspaces $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$, $n = 1, 2, \ldots, \bar{\nu}(\mathbf{r}_0, \mathbf{A})$, can be constructed by the inconsistent* ORTHORES *algorithm, which at the same time produces an approximate solution $\mathbf{x}_n$ whenever the nth basis polynomial t_n has no zero at the origin.*
If the implemented method has the finite termination property, $\mathbf{x}_{\bar{\nu}(\mathbf{r}_0,\mathbf{A})} = \mathbf{x}_\star$.

There is lots of freedom in choosing the basis vectors. In particular they could be chosen orthonormal, in which case the first recursion of the inconsistent ORTHORES algorithm is just the Arnoldi process. So, in this case inconsistent ORTHORES is an alternative to GMRES or FOM, and in the symmetric case as well to MINRES and SYMMLQ. Compared to the classical ORTHORES algorithm of Young and Jea (1980), there are no pivot breakdowns.

Restarts and truncation are possible. But there may be roundoff propagation problems. Of course, in the case of orthogonal residuals, the modified Gram-Schmidt (MGS) formulas should be applied instead of the classical (CGS) ones.

6. Search Directions and Coupled Recursions. In this section we discuss how the Corollaries 4.6 and 4.7 lead to alternative recursions that involve search directions in addition to iterates and residuals.

We assume that the irreducible Hessenberg matrix $\mathbf{H}_m$ is nonsingular and has $m-1$ nonsingular leading principle submatrices. So by a diagonal similarity transformation it can be brought into the form of $\mathbf{H}^\circ_m$, which has zero column sums in all but the last column, which has a nonzero sum. (Recall: otherwise $\mathbf{e}^\mathsf{T}$ were a left eigenvector with the eigenvalue 0.) Equivalently, we could assume that the latter matrix is the given one.

By Corollary 4.6 $\mathbf{H}^\circ_m$ has a Gaussian LU decomposition without pivoting, *i.e.*, $\mathbf{H}^\circ_m = \mathbf{L}^\circ_m\mathbf{U}_m$ with $\mathbf{L}^\circ_m$ nonsingular lower triangular and $\mathbf{U}_m$ unit upper triangular. Then also the extended Hessenberg matrix $\underline{\mathbf{H}}^\circ_m$ has such a decomposition,

$$\underline{\mathbf{H}}^\circ_m = \underline{\mathbf{L}}^\circ_m\mathbf{U}_m\,, \tag{6.1}$$

since we just have to append to $\mathbf{L}^\circ_m$ the last row $\eta^\circ_{m,m-1}\mathbf{l}^\mathsf{T}_m$ of $\underline{\mathbf{H}}^\circ_m$ with $\eta^\circ_{m,m-1} :\equiv -\sum_{k=0}^{m-1}\eta^\circ_{k,m-1}$ $(\neq 0)$.

LEMMA 6.1. *In the decomposition* (6.1) $\underline{\mathbf{L}}_m^\circ$ *is lower bidiagonal and has vanishing column sums, that is, it has the form*

$$\underline{\mathbf{L}}_m^\circ \equiv: \begin{pmatrix} \omega_0^{-1} & & & & \\ -\omega_0^{-1} & \omega_1^{-1} & & & \\ & -\omega_1^{-1} & \omega_2^{-1} & & \\ & & \ddots & \ddots & \\ & & & -\omega_{m-2}^{-1} & \omega_{m-1}^{-1} \\ & & & & -\omega_{m-1}^{-1} \end{pmatrix}. \tag{6.2}$$

PROOF. It is well known and easy to verify that the LU–decomposition of a Hessenberg matrix yields a lower bidiagonal and an upper triangular matrix. The elements on the diagonal of $\mathbf{L}_m^\circ$ are nonzero since $\mathbf{H}_m^\circ$ is assumed to be nonsingular. Furthermore, in view of (4.9) we have

$$\mathbf{e}^{\mathsf{T}}\underline{\mathbf{L}}_m^\circ = \mathbf{e}^{\mathsf{T}}\underline{\mathbf{H}}_m^\circ \mathbf{U}_m^{-1} = \mathbf{o}^{\mathsf{T}}\mathbf{U}_m^{-1} = \mathbf{o}^{\mathsf{T}} . \tag{6.3}$$

□

Let us denote the elements of $\mathbf{U}_m$ by $\psi_{k,n}$:

$$\mathbf{U}_m \equiv: \begin{pmatrix} 1 & \psi_{0,1} & \psi_{0,2} & \cdots & \psi_{0,m-1} \\ & 1 & \psi_{1,2} & \cdots & \psi_{1,m-1} \\ & & 1 & \ddots & \vdots \\ & & & \ddots & \psi_{m-2,m-1} \\ & & & & 1 \end{pmatrix}. \tag{6.4}$$

We now define **search directions** $\mathbf{v}_n$ and a corresponding matrix $\mathbf{V}_m$ by

$$\begin{pmatrix} \mathbf{v}_0 & \mathbf{v}_1 & \cdots & \mathbf{v}_{m-1} \end{pmatrix} :\equiv \mathbf{V}_m :\equiv \mathbf{R}_m \mathbf{U}_m^{-1} , \tag{6.5}$$

so that (4.4), $\mathbf{A}\mathbf{R}_m = \mathbf{R}_{m+1}\underline{\mathbf{H}}_m^\circ$, becomes equivalent to the coupled identities

$$\boxed{\mathbf{R}_m = \mathbf{V}_m \mathbf{U}_m , \qquad \mathbf{A}\mathbf{V}_m = \mathbf{R}_{m+1}\underline{\mathbf{L}}_m^\circ .} \tag{6.6}$$

The second one implies further that the iterates satisfy

$$\boxed{\mathbf{V}_m = -\mathbf{X}_{m+1}\underline{\mathbf{L}}_m^\circ .} \tag{6.7}$$

These three identities are shorthand for the **coupled recursions**

$$\mathbf{v}_n := \mathbf{r}_n - \mathbf{v}_{n-1}\,\psi_{n-1,n} - \cdots - \mathbf{v}_0\,\psi_{0,n} , \tag{6.8a}$$

$$\mathbf{r}_{n+1} := \mathbf{r}_n - \mathbf{A}\mathbf{v}_n\,\omega_n , \tag{6.8b}$$

$$\mathbf{x}_{n+1} := \mathbf{x}_n + \mathbf{v}_n\,\omega_n . \tag{6.8c}$$

The last recursion motivates the name search direction for $\mathbf{v}_n$. Moreover, ω_n is seen to be the **step length**. However, we must admit that, in general, $\mathbf{v}_n$ is neither normalized nor orthogonal.

In summary, we have seen that every Krylov space solver written in the form (4.2)–(4.1) with the condition (4.3) can be reformulated as (6.8a)–(6.8c). The latter version is the ORTHOMIN form of a Krylov space solver. It is a generalization of the ORTHOMIN algorithm of Vinsome (1976), where the search directions are $\mathbf{A}^\star\mathbf{A}$–orthogonal and the residuals are minimal like in GMRES.

ALGORITHM 4 (ORTHOMIN FORM OF A KRYLOV SPACE SOLVER).
The ORTHOMIN *form of a Krylov space method for solving* $\mathbf{A}\mathbf{x} = \mathbf{b}$ *applies the recursions* (6.8a)–(6.8c). *They require an initial approximation* $\mathbf{x}_0$ *and the corresponding residual, which is also the first search direction:* $\mathbf{v}_0 := \mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$. *The coefficients* $\psi_{k,n}$, $(k = 0, \dots, n-1;\ n = 0, \dots, m-1)$ *as well as the step length* ω_n *depend on the particular solver.*

In particular, the step length ω_n is easily chosen so that the residual $\mathbf{r}_{n+1}$ is minimized in some norm on the straight line $\omega \mapsto \mathbf{r}_n + \mathbf{A}\mathbf{v}_n\,\omega_n$.

While the reformulation of a method given only by its coefficients $\eta^\circ_{k,n}$ (that is, by $\underline{\mathbf{H}}^\circ_m$) requires to LU-decompose $\underline{\mathbf{H}}^\circ_m$, the methods based on orthogonal or oblique projection allow us to compute the coefficients of $\underline{\mathbf{L}}^\circ_m$ and $\mathbf{U}_m$ directly.

There is a third basic form for Krylov space solvers, the ORTHODIR form. We obtain it by eliminating from (6.6) the residual vectors:

$$\boxed{\mathbf{A}\mathbf{V}_m = \mathbf{V}_{m+1}\underline{\mathbf{H}}'_m\,, \qquad \text{where} \quad \underline{\mathbf{H}}'_m :\equiv \mathbf{U}_{m+1}\underline{\mathbf{L}}^\circ_m\,.} \tag{6.9}$$

$\underline{\mathbf{H}}'_m$ is again an extended Hessenberg matrix, but its column sums are, in general, not zero.

The identity (6.9) yields a recursion for the search directions, but we need additionally a way to update the iterates, and, preferably, also the residuals, since otherwise we spend two matrix-vector multiplications per step, one to update the search direction and the other for computing the residual (in order to judge the quality of the approximation $\mathbf{x}_n$). The two formulas (6.8b) and (6.8c) satisfy this need. Together with the recursion expressed by (6.9) and given as (6.10a) next, they yield the ORTHODIR form of a method:

ALGORITHM 5 (ORTHODIR FORM OF A KRYLOV SPACE SOLVER).
The ORTHODIR *form of a Krylov space method for solving* $\mathbf{A}\mathbf{x} = \mathbf{b}$ *applies, for* $n = 0, 1, \dots,$ *the recursions*

$$\mathbf{v}_n := \left(\mathbf{A}\mathbf{v}_{n-1} - \mathbf{v}_{n-1}\,\eta'_{n-1,n-1} \cdots - \mathbf{v}_0\,\eta'_{0,n-1}\right)/\eta'_{n,n-1}\,, \tag{6.10a}$$

$$\mathbf{r}_{n+1} := \mathbf{r}_n - \mathbf{A}\mathbf{v}_n\,\omega_n\,, \tag{6.10b}$$

$$\mathbf{x}_{n+1} := \mathbf{x}_n + \mathbf{v}_n\,\omega_n\,. \tag{6.10c}$$

They require an initial approximation $\mathbf{x}_0$ *and the corresponding residual, which is also the first search direction:* $\mathbf{v}_0 := \mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$. *The coefficients* $\eta'_{k,n}$, $(k = 0, \dots, n-1;\ n = 0, 1, \dots, m-1)$ *as well as the step length* ω_n *depend on the particular solver.*

So here the Krylov space is generated by a recursion for the search directions, while in the ORTHORES form it is generates by the recursion for the residual vectors, and in the ORTHOMIN form by two coupled recursions involving both vector sequences. Again, the step length ω_n is normally determined by some minimality or orthogonality condition for the residual.

In summary we have found the following:

THEOREM 6.2. *If the iterates* $\mathbf{x}_n$ *of a Krylov space solver are defined for all* n *up to* m*, then they can be computed*

1) *by an* ORTHORES *algorithm based on the recursions* (4.2)–(4.1) *with the restriction* (4.3) *and the compact form* (4.4)*;*
2) *by an inconsistent* ORTHORES *algorithm based on the recursions* (5.1)–(5.4) *with the compact form* (5.6)–(5.8)*;*
3) *by an* ORTHOMIN *algorithm based on the recursions* (6.8a)–(6.8c) *with the compact form* (6.6)–(6.7)*;*
4) *by an* ORTHODIR *algorithm based on the recursions* (6.10a)–(6.10c) *with the compact form consisting of the right-hand side relation in* (6.6)*, of* (6.7)*, and* (6.9)*.*

In contrast to the other methods the inconsistent ORTHORES *algorithm still works if some* $\mathbf{x}_{n+1}$ *is undefined (or infinite) due to* $t_{n+1}(0) = 0$*. On the other hand, the* ORTHOMIN *and* ORTHODIR *algorithms also work if* $\mathbf{x}_{n+1}$ *stagnates due to* $\omega_n = 0$*, in which case* p_{n+1} *does not have full degree* n*.*

In general, in any of the three forms, a Krylov space method may have the disadvantage to require the storage of all previous iterates, all previous residuals, or all previous search directions. However, we know from the CG and CR methods, that there are situations where this is not the case. Here is a related result:

THEOREM 6.3. *Under the assumption of Theorem 6.2, the following three statements are equivalent with some* $\ell \geq 0$*:*

1) *In the* ORTHORES *algorithm the recursions for the residuals and iterates are at most* $\ell + 2$*-term:*

$$\begin{aligned} \mathbf{r}_{n+1} &:= \left(\mathbf{A}\mathbf{r}_n - \mathbf{r}_n\,\eta^\circ_{n,n} - \cdots - \mathbf{r}_{n-\ell}\,\eta^\circ_{n-\ell,n} -\right) / \eta^\circ_{n+1,n}\,, \\ \mathbf{x}_{n+1} &:= -\left(\mathbf{r}_n + \mathbf{x}_n\,\eta^\circ_{n,n} + \cdots + \mathbf{x}_{n-\ell}\,\eta^\circ_{n-\ell,n}\right) / \eta^\circ_{n+1,n}\,; \end{aligned}$$

2) *In the inconsistent* ORTHORES *algorithm the recursions for* $\mathbf{y}_n$ *and* $\widehat{\mathbf{x}}_n$ *are at most* $\ell + 2$*-term:*

$$\begin{aligned} \mathbf{y}_{n+1} &:= \left(\mathbf{A}\mathbf{y}_n - \mathbf{y}_n\,\eta_{n,n} - \cdots - \mathbf{y}_{n-\ell}\,\eta_{n-\ell,n} -\right) / \eta_{n+1,n}\,, \\ \widehat{\mathbf{x}}_{n+1} &:= -\left(\mathbf{y}_n + \widehat{\mathbf{x}}_n\,\eta_{n,n} + \cdots + \widehat{\mathbf{x}}_{n-\ell}\,\eta_{n-\ell,n}\right) / \eta_{n+1,n}\,; \end{aligned}$$

3) *In the* ORTHOMIN *algorithm the recursions for the search directions are at most* $\ell + 1$*-term:*

$$\begin{aligned} &\mathbf{v}_n := \mathbf{r}_n - \mathbf{v}_{n-1}\,\psi_{n-1,n} - \cdots - \mathbf{v}_{n-\ell}\,\psi_{n-\ell,n} \qquad \text{if} \quad \ell > 0\,, \\ &\mathbf{v}_n := \mathbf{r}_n \qquad \text{if} \quad \ell = 0\,, \end{aligned}$$

4) *In the* ORTHODIR *algorithm the recursions for the search directions are at most* $\ell + 2$*-term:*

$$\mathbf{v}_n := \left(\mathbf{A}\mathbf{v}_{n-1} - \mathbf{v}_{n-1}\,\eta'_{n-1,n-1} - \cdots \mathbf{v}_{n-\ell-1}\,\eta'_{n-\ell-1,n-1}\right) / \eta'_{n,n-1}\,.$$

PROOF. The first two statements are equivalent because the sequences $\{\mathbf{y}_n\}$ and $\{\mathbf{r}_n\}$ as well as $\{\widehat{\mathbf{x}}_n\}$ and $\{\mathbf{x}_n\}$ are related by (5.4). The first and the third statements are equivalent because the LU decomposition of a banded Hessenberg matrix $\mathbf{H}^\circ_m$ with upper bandwidth $\ell \geq 0$ yields a lower bidiagonal matrix $\mathbf{L}^\circ_m$ and an upper triangular matrix $\mathbf{U}_m$ with upper bandwidth ℓ — and vice versa. Moreover, since the same is true for the UL decomposition in (6.9), the third and the fourth statement are also equivalent. □

7. A More General Framework. Instead of the nested Krylov spaces $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ that were the starting point for our definition of a Krylov space solver in (2.3), we consider a more general situation and let $\{\mathcal{L}_n\}_{n=1}^{\nu}$ be any finite sequence of nested subspaces with $\mathsf{dim}\ \mathcal{L}_n = n$ for $n \leq \nu$. In other words,

$$\boxed{\mathcal{L}_n :\equiv \mathsf{span}\,\{\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{n-1}\}} \tag{7.1}$$

with a sequence $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{\nu-1}$ of linearly independent vectors. We further assume that

$$\boxed{\mathbf{x}_n - \mathbf{x}_0 \in \mathcal{L}_n \backslash \mathcal{L}_{n-1}} \qquad (n = 1, \ldots, \nu)\,. \tag{7.2}$$

So the errors $\mathbf{d}_n :\equiv \mathbf{x}_n - \mathbf{x}_\star$ and the residuals $\mathbf{r}_n :\equiv \mathbf{b} - \mathbf{A}\mathbf{x}_n$ associated with $\mathbf{x}_n$ still satisfy $\mathbf{r}_n = -\,\mathbf{A}\mathbf{d}_n$ and additionally

$$\mathbf{d}_n - \mathbf{d}_0 \in \mathcal{L}_n \backslash \mathcal{L}_{n-1}\,, \qquad \mathbf{r}_n - \mathbf{r}_0 \in \mathbf{A}\mathcal{L}_n \backslash \mathbf{A}\mathcal{L}_{n-1}\,. \tag{7.3}$$

Using as before the notation $\mathbf{Y}_m :\equiv \begin{pmatrix} \mathbf{y}_0 & \cdots & \mathbf{y}_{m-1} \end{pmatrix}$, $\mathbf{X}_m :\equiv \begin{pmatrix} \mathbf{x}_0 & \cdots & \mathbf{x}_{m-1} \end{pmatrix}$, $\mathbf{R}_m :\equiv \begin{pmatrix} \mathbf{r}_0 & \cdots & \mathbf{r}_{m-1} \end{pmatrix}$, we get the following result analogous to Theorem 4.1:

THEOREM 7.1. *If defined for all n up to m $(\leq \nu)$, the iterates $\mathbf{x}_n$ and the corresponding residuals $\mathbf{r}_n$ of a linear solver characterized by (7.2) satisfy, for $n = 0, 1, \ldots, m-1$,*

$$\mathbf{x}_{n+1} := -\left(\mathbf{y}_n + \mathbf{x}_n\, \eta^\circ_{n,n} + \cdots + \mathbf{x}_0\, \eta^\circ_{0,n}\right) / \eta^\circ_{n+1,n}\,, \tag{7.4a}$$

$$\mathbf{r}_{n+1} := \left(\mathbf{A}\mathbf{y}_n - \mathbf{r}_n\, \eta^\circ_{n,n} - \cdots - \mathbf{r}_0\, \eta^\circ_{0,n}\right) / \eta^\circ_{n+1,n}\,, \tag{7.4b}$$

where $\eta^\circ_{n+1,n} :\equiv -\,\eta^\circ_{n,n} - \cdots - \eta^\circ_{0,n}$. Equivalently, in matrix form,

$$\boxed{\mathbf{Y}_m = -\mathbf{X}_{m+1}\underline{\mathbf{H}}^\circ_m\,, \qquad \mathbf{A}\mathbf{Y}_m = \mathbf{R}_{m+1}\underline{\mathbf{H}}^\circ_m} \tag{7.5}$$

with a full rank $(m+1) \times m$ Hessenberg matrix $\underline{\mathbf{H}}^\circ_m$ with column sums 0.

Note that in contrast to (4.4) in Theorem 4.1 the matrices $\mathbf{Y}_m$ and $\mathbf{R}_m$ are different here, and this, in general, by more than the scaling of the columns. We will refer to this solver as the **generalized** ORTHORES **algorithm**.

PROOF of Theorem 7.1 The proof is analogous to that of Theorem 4.1. By assumption (7.2) holds, so with the matrix $\underline{\mathbf{F}}_m$ from (4.5) we have now

$$\mathbf{X}_{m+1}\underline{\mathbf{F}}_m = -\mathbf{Y}_m\mathbf{U}_m \tag{7.6}$$

with a nonsingular upper triangular $m \times m$ matrix $\mathbf{U}_m$. Again $\begin{pmatrix} \mathbf{b} & \mathbf{b} & \cdots & \mathbf{b} \end{pmatrix}\underline{\mathbf{F}}_m = \mathbf{b}\mathbf{e}^\mathsf{T}\underline{\mathbf{F}}_m = \mathbf{O}$. Therefore,

$$\begin{aligned} \mathbf{R}_{m+1}\underline{\mathbf{F}}_m &= \left(\begin{pmatrix} \mathbf{b} & \cdots & \mathbf{b} \end{pmatrix} - \mathbf{A}\mathbf{X}_{m+1}\right)\underline{\mathbf{F}}_m \\ &= -\mathbf{A}\mathbf{X}_{m+1}\underline{\mathbf{F}}_m = \mathbf{A}\mathbf{Y}_m\mathbf{U}_m\,. \end{aligned} \tag{7.7}$$

So, with $\underline{\mathbf{H}}^\circ_m :\equiv \underline{\mathbf{F}}_m\mathbf{U}_m^{-1}$ as in (7.5) we can write (7.6) and (7.7) as (4.4), where $\underline{\mathbf{H}}^\circ_m$ is an $(m+1) \times m$ upper Hessenberg matrix that satisfies $\mathbf{e}^\mathsf{T}\underline{\mathbf{H}}^\circ_m = \mathbf{o}^\mathsf{T}$. $\square$

There are some widely used methods that fit into this framework, but not in the one of standard Krylov space solvers treated before.

One class are block Krylov space methods, where the subspaces $\mathcal{L}_m$ are direct sums of Krylov subspaces of the form $\mathcal{K}_{n_k}(\mathbf{A}, \mathbf{r}_{0,k})$, some of which may already be exhausted (*i.e.*, $n_k \geq \bar{\nu}(\mathbf{r}_{0,k}, \mathbf{A})$), while others are still growing.

Another case of importance is when the search space is essentially a Krylov space generated by a matrix $\mathbf{B}$ different from $\mathbf{A}$. One encounters this case when treating least squares problems with the CGNR and CGNE algorithms. More specifically, we consider the nested spaces

$$\boxed{\mathcal{L}_n :\equiv \mathbf{A}^{-1}\mathbf{B}\mathcal{K}_n(\mathbf{B}, \mathbf{r}_0) = \mathsf{span}\,\{\mathbf{A}^{-1}\mathbf{B}\,\mathbf{r}_0, \mathbf{A}^{-1}\mathbf{B}^2\mathbf{r}_0, \ldots, \mathbf{A}^{-1}\mathbf{B}^n\mathbf{r}_0\}\,.} \tag{7.8}$$

Then, in the recursions (7.4a)–(7.4b) we can choose

$$\boxed{\mathbf{y}_n :\equiv \mathbf{A}^{-1}\mathbf{B}\,\mathbf{r}_n\,,} \tag{7.9}$$

so that they become

$$\mathbf{x}_{n+1} := -\left(\mathbf{A}^{-1}\mathbf{B}\,\mathbf{r}_n + \mathbf{x}_n\,\eta^\circ_{n,n} + \mathbf{x}_{n-1}\,\eta^\circ_{n-1,n} + \cdots + \mathbf{x}_0\,\eta^\circ_{0,n}\right)/\eta^\circ_{n+1,n}\,, \tag{7.10a}$$

$$\mathbf{r}_{n+1} := \left(\mathbf{B}\,\mathbf{r}_n - \mathbf{r}_n\,\eta^\circ_{n,n} - \mathbf{r}_{n-1}\,\eta^\circ_{n-1,n} - \cdots - \mathbf{r}_0\,\eta^\circ_{0,n}\right)/\eta^\circ_{n+1,n}\,, \tag{7.10b}$$

or, in compact form, since $\mathbf{Y}_m = \mathbf{A}^{-1}\mathbf{B}\,\mathbf{R}_m$,

$$\boxed{\mathbf{A}^{-1}\mathbf{B}\,\mathbf{R}_m = -\mathbf{X}_{m+1}\underline{\mathbf{H}}^\circ_m\,, \qquad \mathbf{B}\mathbf{R}_m = \mathbf{R}_{m+1}\underline{\mathbf{H}}^\circ_m\,.} \tag{7.11}$$

Of course, this make sense only if matrix-vector products of the form $\mathbf{A}^{-1}\mathbf{B}\,\mathbf{r}$ can be computed easily, as, *e.g.*, in the cases where $\mathbf{B} = \mathbf{A}$ or $\mathbf{B} = \mathbf{A}\mathbf{A}^\star$. The first case, $\mathbf{B} = \mathbf{A}$, is the standard situation treated before, where these recursions reduce to (4.2)–(4.1) with the compact representation (4.4). The second case, $\mathbf{B} = \mathbf{A}\mathbf{A}^\star$, is what we encounter in the CGNR and CGNE algorithms.

As before, the Hessenberg matrix $\underline{\mathbf{H}}^\circ_m$ (with zero column sums) of Theorem 7.1 has an LU decomposition $\underline{\mathbf{H}}_m = \underline{\mathbf{L}}_m\mathbf{U}_m$; see Theorem 4.4 and Corollary 4.7. The factors $\underline{\mathbf{L}}_m$ and $\mathbf{U}_m$ can be taken of the same forms as in (6.2) and (6.4).

This leads quickly to a **generalized** ORTHOMIN **algorithm**: We define the **search directions** $\mathbf{v}_n$ and a corresponding matrix $\mathbf{V}_m$ again by

$$\begin{pmatrix} \mathbf{v}_0 & \mathbf{v}_1 & \cdots & \mathbf{v}_{m-1} \end{pmatrix} :\equiv \mathbf{V}_m :\equiv \mathbf{R}_m\mathbf{U}_m^{-1}\,, \tag{7.12}$$

so that (4.4), $\mathbf{A}\mathbf{Y}_m = \mathbf{R}_{m+1}\underline{\mathbf{H}}^\circ_m$, becomes equivalent to the coupled identities

$$\boxed{\mathbf{Y}_m = \mathbf{V}_m\mathbf{U}_m\,, \qquad \mathbf{A}\mathbf{V}_m = \mathbf{R}_{m+1}\underline{\mathbf{L}}^\circ_m\,.} \tag{7.13}$$

The second one implies further that the iterates satisfy

$$\boxed{\mathbf{V}_m = -\mathbf{X}_{m+1}\underline{\mathbf{L}}^\circ_m\,.} \tag{7.14}$$

These three identities are shorthand for the **generalized coupled recursions**

$$\mathbf{v}_n := \mathbf{y}_n - \mathbf{v}_{n-1}\,\psi_{n-1,n} - \cdots - \mathbf{v}_0\,\psi_{0,n}\,, \tag{7.15a}$$

$$\mathbf{r}_{n+1} := \mathbf{r}_n - \mathbf{A}\mathbf{v}_n\,\omega_n\,, \tag{7.15b}$$

$$\mathbf{x}_{n+1} := \mathbf{x}_n + \mathbf{v}_n\,\omega_n\,. \tag{7.15c}$$

Since the residuals appear now only in one of the two equations (7.13) there is no way to eliminate them in order to define a generalized ORTHODIR version in the same way as before.

There is also no easy way to define a generalized inconsistent ORTHORES algorithm.

8. Conclusions. We have shown that under very mild conditions every Krylov space solver has realizations based on general OrthoMin, OrthoRes, and OrthoDir recurrences, which are generalizations of the classical OrthoMin, OrthoRes, and OrthoDir recurrences of Vinsome (1976) and Young and Jea (1980), but do not assume any orthogonality of the residuals or of the search directions, in contrast to the classical algorithms, which were designed for orthogonal residual and minimum residual methods. While OrthoRes is based on a recurrence for the residuals, the recurrences of OrthoMin and OrthoDir involve both residuals and search directions (direction vectors). We have established various equivalent conditions for the validity of these recurrences, one being that so-called pivot breakdowns do not happen. We have also introduced a general algorithm, inconsistent OrthoRes, which does not suffer from such pivot breakdowns. It computes, in each step, an approximation of the solution of a linear system whose right-hand side $\mathbf{b}$ is suitably scaled.

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