

Approximately invariant subspaces

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Abstract

Invariant subspaces are well documented in the literature and approximations for them exist. Approximately invariant subspaces have properties that are highly desirable for iterative solution strategies of large sparse matrix systems and for approximating Ritz values and Ritz vectors of such matrices. It is often a difficult task to identify an approximately invariant subspace numerically. In this work a new definition is proposed that assists with the task of identifying when a subspace is approximately invariant by measuring the sine of the angle between the image of any vector in the subspace and its orthogonal projection onto the subspace. In particular the effect that different bases have on this measure is analysed. Finally, the definition is used to provide theoretical error estimates when solving either systems of equations or the eigenvalue problem.

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1 Introduction

The solution of a system of linear equations $\mathbf{Ax} = \mathbf{b}$, when the $n \times n$ coefficient matrix \mathbf{A} is large and sparse is of considerable interest in a variety of applications in science and technology. The most popular iterative techniques utilise Krylov methods to construct a subspace on which the solution can be approximated. If \mathbf{A} is nonsingular, the system has a unique solution $\mathbf{x} \in \mathcal{K}_m(\mathbf{A}, \mathbf{b}) = \text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \dots, \mathbf{A}^{m-1}\mathbf{b}\}$, where m is the algebraic grade,

namely the degree of the minimal polynomial of \mathbf{A} . For matrices that are diagonalisable, m is the number of distinct eigenvalues and may range from 1 to n . If m is small, the *Arnoldi* decomposition, or *Lanczos* method for symmetric matrices, converges rapidly as implemented in GMRES(k) [1, 2] or MINRES [4]. The criterion for terminating the sequence is to monitor the norm of the residual $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$.

There are, as with any iterative methods, some drawbacks in implementing a Krylov method and these should be mentioned. If \mathbf{A} is singular, Krylov methods can fail, even if the system has a solution [3]. If \mathbf{A} is a Jordan Block of order n , then $m = n$, which is not a practical option since the residual may not converge to zero until n iterations [3]. Furthermore, as far as can be ascertained from the literature for GMRES-type algorithms, some value for k in GMRES(k) is arbitrarily chosen for restarting the process in order to reduce computational difficulties that may arise when dealing with large dimensional Krylov subspaces, including for example, large memory requirements and potential loss of orthogonality in the orthonormal basis. However, in many cases, after a certain number of restarts, the small reductions encountered in the residual may not justify the expanded work. From the experience of the authors, there appears to be an optimal value, which here will be referred to as the *analytic grade* ℓ that provides approximately the same result as $k \gg \ell$ but is well short of m . This concept is introduced in terms of approximately invariant subspaces and will be elaborated on in future research.

In the next section of this paper (§2) a solution methodology is analysed that enables the problem $\mathbf{A}\mathbf{x} = \mathbf{b}$ in \mathbb{R}^n to be reduced to a more tractable problem $\hat{\mathbf{A}}\mathbf{y} = \mathbf{z}$ on a low dimensional subspace. Then (§§3–4) the notion of approximately invariant subspaces as required for this study is discussed. This concept is not new [5] but

the approach proposed here is believed to be more direct because it helps answer the question of how the choice of the basis affects the error in solving the system of equations or the algebraic eigenvalue problem. The following Section 5 examines theoretical error bounds on these two standard numerical linear algebra problems and then two case studies are provided (§6) that assess the proposed theory. Finally (§7), the main conclusions of the work are summarised.

2 Solution methodology

Let \mathbf{A} be a large sparse $n \times n$ matrix. Clearly in this case it is not practical to solve the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ using classical direct or indirect methods. A better strategy is to try to construct a low dimensional subspace that captures \mathbf{b} sufficiently well to yield an approximate solution.

The best known techniques for achieving this objective are the *projection methods* or *Galerkin methods* [2]. For easier exposition we have exhibited these methods schematically in Figure 1. The matrices $\bar{\mathbf{A}}$ and $\hat{\mathbf{A}}$ are defined from the diagram, which we now explain.

Given an m -dimensional subspace $V \subset \mathbb{R}^n$ and a k -dimensional ($k \leq m$) subspace $W \subset \mathbb{R}^n$, let the $n \times m$ matrix $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_m]$ have the basis vectors for V as its columns and the $n \times k$ matrix $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_k]$ for W . It is useful to take \mathbf{V} and \mathbf{W} not necessarily ON as is done with the Krylov basis in Section 6. Let \mathbf{V}^L and \mathbf{W}^L denote the left inverses of \mathbf{V} and \mathbf{W} respectively. The transformation $\bar{\mathbf{A}} : V \rightarrow W$ is defined from the diagram as $\bar{\mathbf{A}}\mathcal{P}_V\mathbf{x} = \mathcal{P}_W\mathbf{A}\mathbf{x}$, for all $\mathbf{x} \in \mathbb{R}^n$, so that $\bar{\mathbf{A}}\mathcal{P}_V = \mathcal{P}_W\mathbf{A}$. From the figure see that $\mathbf{v} = \mathcal{P}_V\mathbf{x} = \mathbf{V}\mathbf{y}$. Both $\bar{\mathbf{A}}\mathbf{v} = \bar{\mathbf{A}}\mathbf{V}\mathbf{y} = \bar{\mathbf{A}}\mathcal{P}_V\mathbf{V}\mathbf{y}$ and $\mathbf{w} = \mathcal{P}_W\mathbf{b}$ are contained in W , which enables the solution to be found in \mathbb{R}^k using the left

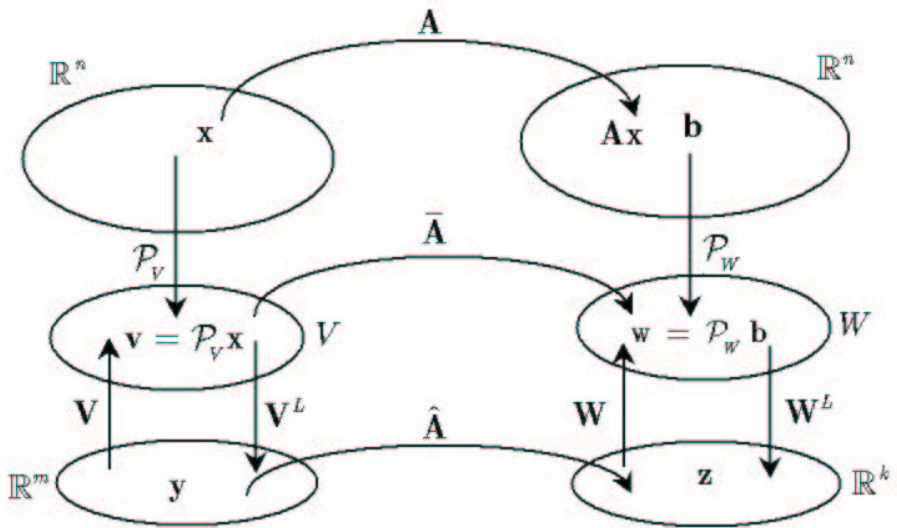


FIGURE 1: Construction of a low dimensional subspace

inverse of \mathbf{W} :

$$\mathbf{W}^L \bar{\mathbf{A}} \mathcal{P}_V \mathbf{V} \mathbf{y} = \mathbf{z} = \mathbf{W}^L \mathcal{P}_W \mathbf{b}.$$

Again from the diagram $\bar{\mathbf{A}} \mathbf{V} \mathbf{y} = \mathbf{W} \hat{\mathbf{A}} \mathbf{y}$, for all $\mathbf{y} \in \mathbb{R}^m$ so that $\bar{\mathbf{A}} \mathbf{V} = \mathbf{W} \hat{\mathbf{A}}$. Since $\mathbf{v} = \mathcal{P}_V \mathbf{v}$, the above system becomes

$$\hat{\mathbf{A}} \mathbf{y} = \mathbf{z}, \quad (1)$$

where $\hat{\mathbf{A}} = \mathbf{W}^L \mathcal{P}_W \mathbf{A} \mathbf{V} = \mathbf{W}^L \mathbf{A} \mathbf{V}$ and $\mathbf{z} = \mathbf{W}^L \mathcal{P}_W \mathbf{b} = \mathbf{W}^L \mathbf{b}$ as explained below. If $\mathbf{W} = \mathbf{Q} \mathbf{R}$ is the QR decomposition of \mathbf{W} , $\mathcal{P}_W = \mathbf{Q} \mathbf{Q}^T$ and $\mathbf{W}^L = \mathbf{R}^{-1} \mathbf{Q}^T$ is the left inverse of \mathbf{W} . A key observation is that $\mathbf{W}^L \mathcal{P}_W = \mathbf{R}^{-1} \mathbf{Q}^T \mathbf{Q} \mathbf{Q}^T = \mathbf{R}^{-1} \mathbf{Q}^T = \mathbf{W}^L$, so that one can interpret the effect of \mathbf{W}^L as first a projection onto W followed by inversion to \mathbb{R}^k . Not surprisingly equation (1) is the same as would result by using the *Petrov-Galerkin* projection $\mathbf{W}^L (\mathbf{b} - \mathbf{A} \mathbf{V} \mathbf{y}) = \mathbf{0}$.

The solution $\mathbf{x} = \mathbf{V} \mathbf{y}$, where \mathbf{y} satisfies (1), or equivalently

$$\mathbf{Q}^T \mathbf{A} \mathbf{V} \mathbf{y} = \mathbf{Q}^T \mathbf{b},$$

is the least squares solution on V of $\mathbf{A} \mathbf{x} = \mathbf{b}$. If $\mathbf{b} \in W$, the solution is exact; otherwise, the relative error is $\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\| / \|\mathbf{b}\|$, where \mathcal{P}_W is the projection onto W . This relative error in effect measures the relative residual of the least squares solution on V , if (1) can be solved exactly.

In constructing the subspaces V and W , one has the primary aim in mind to capture $\mathbf{b} \in W$, giving rise to:

Test 1 Is $\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\| / \|\mathbf{b}\| < \varepsilon$ for a given ε ?

If V can be found of low dimensionality such that \mathbf{b} satisfies Test 1, it is easy to obtain the solution of the linear system.

The eigenvalue problem $\mathbf{Ax} = \lambda\mathbf{x}$ can be treated in the same way. From the diagram (take $W = V$) $\bar{\mathbf{A}}\mathcal{P}_V\mathbf{x} = \mathcal{P}_V\mathbf{Ax} = \lambda\mathcal{P}_V\mathbf{x}$, that is, $\bar{\mathbf{A}}\mathbf{Vy} = \lambda\mathbf{Vy}$, that is, $\hat{\mathbf{A}}\mathbf{y} = \lambda\mathbf{y}$, where $\hat{\mathbf{A}} = \mathbf{V}^L\mathbf{AV}$. The solution of the eigenvalue problem $\hat{\mathbf{A}}\mathbf{y} = \theta\mathbf{y}$ approximates the solution of $\mathbf{Ax} = \lambda\mathbf{x}$, that is, θ approximates λ and $\mathbf{x} = \mathbf{Vy}$ the corresponding eigenvector. The pair (θ, \mathbf{x}) is known as the Ritz pair of \mathbf{A} on V . Again this result is just the *Ritz-Galerkin* projection method $\mathbf{V}^L(\mathbf{AVy} - \lambda\mathbf{Vy}) = \mathbf{0}$.

2.1 Potential problems with this solution methodology when using $V = \mathcal{K}_m(\mathbf{b}, \mathbf{A})$

- If \mathbf{A} is singular, Krylov methods can fail, even if the system has a solution and m is the algebraic grade [3]. Although $W = A(V) \subset V$, $\mathbf{b} \notin W$.
- Even if \mathbf{A} is nonsingular, Krylov methods may still fail to satisfy Test 1 for sufficiently small ε if m is less than the algebraic grade. Although V and W overlap it still may be that W does not capture \mathbf{b} .
- How does one decide on the size of m ?

3 Invariant subspaces

If V is an invariant subspace of \mathbf{A} , that is, $\mathbf{Ax} \in V$ for all $\mathbf{x} \in V$ or $W \subseteq V$, and if \mathbf{A} is nonsingular, then $W = V$. The methodology presented above is simplified considerably and all that is required to devise an efficient numerical strategy for solving a large sparse matrix system is to capture \mathbf{b} in V . However, ensuring that \mathbf{b} is

contained in an invariant subspace V is not straightforward and still remains one of the grand challenges of current worldwide research in such solution strategies. Equation (1) when V is an invariant subspace becomes

$$\mathbf{V}^L \mathbf{A} \mathbf{V} \mathbf{y} = \mathbf{V}^L \mathbf{b}.$$

If $\mathbf{b} \in V$, one easily finds an exact solution. If \mathbf{A} is singular, then even if $\mathbf{b} \in V$, \mathbf{b} may not be in W and there is no guarantee that $\mathbf{A} \mathbf{x} = \mathbf{b}$ will have a solution in V .

On the other hand if one is considering the algebraic eigenvalue problem $\mathbf{A} \mathbf{x} = \lambda \mathbf{x}$ on an invariant subspace V one can always find eigenpairs $(\lambda, \mathbf{x} = \mathbf{V} \mathbf{y})$ of \mathbf{A} on V by solving

$$\mathbf{V}^L \mathbf{A} \mathbf{V} \mathbf{y} = \lambda \mathbf{y}.$$

Note: If V is invariant, then $\mathbf{A} \mathbf{V} = \mathbf{V} \hat{\mathbf{A}}$. Some examples of invariant subspaces of \mathbf{A} are:

1. $\{\mathbf{0}\}$;
2. \mathbb{R}^n ;
3. *nullspace* $\mathcal{N}(\mathbf{A})$;
4. *range* $\mathcal{R}(\mathbf{A})$;
5. *Krylov subspace* $\mathcal{K}_m(\mathbf{A}, \mathbf{b})$ with m the algebraic grade;
6. *eigenspace* belonging to eigenvalue λ ;
7. *span* of a subset of eigenvectors of \mathbf{A} .

4 Approximately invariant subspaces

In general it is hard to detect a fully invariant subspace and as a consequence, an approximation is constructed. This approximation is motivated by the idea that if \mathbf{b} is close to subspace W then $\sin \theta = \|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\|/\|\mathbf{b}\|$ must be small, where θ is the angle between \mathbf{b} and its projection onto W .

This concept leads to the following definition, which tests all vectors in the subspace to identify an approximately invariant subspace. Unless otherwise stated, $\|\cdot\| = \|\cdot\|_2$.

Definition 2 Let $\mathbf{A} : V \rightarrow W$ where V is a subspace of \mathbb{R}^n and $W = \mathbf{A}(V) \subset \mathbb{R}^n$. If

$$\max_{\substack{\mathbf{x} \in V \\ \mathbf{Ax} \neq \mathbf{0}}} \frac{\|\mathbf{Ax} - \mathcal{P}_V(\mathbf{Ax})\|}{\|\mathbf{Ax}\|} < 10^{-t} = \varepsilon, \quad (2)$$

V is defined as an approximately invariant subspace of A of order t (or ε).

This definition is equivalent to

$$\max_{\substack{\mathbf{w} \in W \\ \mathbf{w} \neq \mathbf{0}}} \frac{\|\mathbf{w} - \mathcal{P}_V(\mathbf{w})\|}{\|\mathbf{w}\|} = \sin \theta < \varepsilon, \quad (3)$$

where θ is the angle between \mathbf{w} and its projection onto V . Clearly, if V is an approximately invariant subspace, then every basis of V satisfies (2). The converse, as seen in the following Lemma, is only partially true.

Lemma 3 *If there exists a basis $\{\mathbf{u}_i\}_1^m$ of V such that*

$$\frac{\|\mathbf{A}\mathbf{u}_i - \mathcal{P}_V(\mathbf{A}\mathbf{u}_i)\|}{\|\mathbf{A}\mathbf{u}_i\|} < 10^{-t} = \delta, \quad i = 1, \dots, m,$$

then V is an approximately invariant subspace of \mathbf{A} of order $\varepsilon = \|\mathbf{A}\| \sqrt{m} \delta / \mu_0$, where μ_0 is the smallest singular value of $\mathbf{A}\mathbf{U}$, $\mathbf{U} = [\hat{\mathbf{u}}_1, \dots, \hat{\mathbf{u}}_m]$.

Proof: Without loss of generality, assume \mathbf{u}_i are normalised, that is, $\|\mathbf{u}_i\| = 1$. Any $\mathbf{x} \in V$ can be written as $\mathbf{x} = \sum_{i=1}^m c_i \mathbf{u}_i = \mathbf{U}\mathbf{c}$, $\mathbf{A}\mathbf{x} = \sum_{i=1}^m c_i \mathbf{A}\mathbf{u}_i$. Now (exclude $\mathbf{A}\mathbf{x} = \mathbf{0}$),

$$\begin{aligned} \frac{\|\mathbf{A}\mathbf{x} - \mathcal{P}_V(\mathbf{A}\mathbf{x})\|}{\|\mathbf{A}\mathbf{x}\|} &= \frac{\|\sum_{i=1}^m c_i (\mathbf{A}\mathbf{u}_i - \mathcal{P}_V(\mathbf{A}\mathbf{u}_i))\|}{\|\mathbf{A}\mathbf{x}\|} \\ &\leq \frac{\sum_{i=1}^m |c_i| \|\mathbf{A}\mathbf{u}_i\| \delta}{\|\mathbf{A}\mathbf{x}\|} \\ &\leq \|\mathbf{A}\| \delta \frac{\sum_{i=1}^m |c_i|}{\|\mathbf{A}\mathbf{x}\|} \\ &\leq \|\mathbf{A}\| \delta \sqrt{m} \frac{\|\mathbf{c}\|_2}{\|\mathbf{A}\mathbf{U}\mathbf{c}\|_2} \end{aligned}$$

where $\sum_{i=1}^m |c_i| = \|\mathbf{c}\|_1 \leq \sqrt{m} \|\mathbf{c}\|_2$. Hence,

$$\max_{\mathbf{x} \in V, \mathbf{A}\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x} - \mathcal{P}_V(\mathbf{A}\mathbf{x})\|}{\|\mathbf{A}\mathbf{x}\|} \leq \frac{\|\mathbf{A}\| \sqrt{m}}{\mu_0} \delta,$$

with μ_0 the smallest singular value of $\mathbf{A}\mathbf{U}$. ♠

Notes:

- The hypothesis of Lemma 3 can read: Let $\{\mathbf{u}_i\}_1^m$ be a basis of V . If there exists constants b_{ij} such that

$$\frac{\left\| \mathbf{A}\mathbf{u}_i - \sum_{j=1}^m b_{ij}\mathbf{u}_j \right\|}{\|\mathbf{A}\mathbf{u}_i\|} < 10^{-t} = \varepsilon, \quad i = 1, \dots, m,$$

then V is an approximately invariant subspace of \mathbf{A} of order $\varepsilon = \|\mathbf{A}\| \sqrt{m}\delta/\mu_0$. The reason for this restatement is the well known result

$$\|\mathbf{A}\mathbf{u}_i - \mathcal{P}_V(\mathbf{A}\mathbf{u}_i)\| \leq \left\| \mathbf{A}\mathbf{u}_i - \sum_{j=1}^m b_{ij}\mathbf{u}_j \right\| \quad \text{for all } b_{ij}.$$

- Changing the basis in Lemma 3 will result in a different δ . Thus, using one basis may lead to a conclusion that the space is approximately invariant that could not be detected using another basis.

The discussion of inexact invariant subspaces given by [5] follows from this Lemma 4.

Lemma 4 *Let $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_m]$ be an ON basis of an approximately invariant subspace V of \mathbf{A} of order ε . Then there exists matrices \mathbf{M} and \mathbf{S} such that*

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{M} + \mathbf{S}$$

with the properties:

1. $\mathbf{M} = \mathbf{V}^T \mathbf{A} \mathbf{V}$;
2. $\mathbf{V}^T \mathbf{S} = \mathbf{0}$; and
3. $\|\mathbf{S}\|_2 \leq \|\mathbf{A}\|_2 \varepsilon$.

Proof: By the orthogonal decomposition theorem

$$\mathbf{A}\mathbf{v}_i = \mathcal{P}_V(\mathbf{A}\mathbf{v}_i) + \mathbf{s}_i,$$

where $\mathbf{s}_i \perp V$, that is, $\mathbf{V}^T \mathbf{s}_i = \mathbf{0}$. Now $\mathcal{P}_V(\mathbf{A}\mathbf{v}_i) = \mathbf{V}\mathbf{V}^T \mathbf{A}\mathbf{v}_i$, so that $\mathbf{A}\mathbf{v}_i = \mathbf{V}\mathbf{V}^T \mathbf{A}\mathbf{v}_i + \mathbf{s}_i$. In matrix form, $\mathbf{A}\mathbf{V} = \mathbf{V}(\mathbf{V}^T \mathbf{A}\mathbf{V}) + \mathbf{S}$ which proves 1 and 2. For 3:

$$\begin{aligned} \|\mathbf{S}\|_2 &= \sup_{\mathbf{y} \neq \mathbf{0}} \frac{\|\mathbf{S}\mathbf{y}\|_2}{\|\mathbf{y}\|_2} \\ &= \sup_{\mathbf{y} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{V}\mathbf{y} - \mathbf{V}\mathbf{V}^T \mathbf{A}\mathbf{V}\mathbf{y}\|_2}{\|\mathbf{y}\|_2} \\ &= \sup_{\mathbf{y} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{v} - \mathcal{P}_V(\mathbf{A}\mathbf{v})\|_2}{\|\mathbf{A}\mathbf{v}\|_2} \frac{\|\mathbf{A}\mathbf{V}\mathbf{y}\|_2}{\|\mathbf{y}\|_2} \\ &\leq \varepsilon \|\mathbf{A}\|_2, \quad \text{where } \mathbf{v} = \mathbf{V}\mathbf{y}. \end{aligned}$$



5 Error bounds

In this section theoretical error bounds will be derived for the residuals associated with the solution of large sparse, linear system and the algebraic eigenvalue problem. In a perfect world these bounds would be sufficient to complete the treatise of solving these two problems on approximately invariant subspaces. Unfortunately, in the computational world other sources of error manifest and this section finishes with a brief discussion of potential inaccuracies that can arise with the theoretical error bounds given below in Theorems 5 and 6, including the impact of floating point arithmetic.

An estimate for the error in Test 1 is given by the following theorem.

Theorem 5 Let V be an approximately invariant subspace of a nonsingular matrix \mathbf{A} of order δ with ON basis $\{\mathbf{v}_i\}$ and $\mathbf{W} = \mathbf{A}\mathbf{V}$. If $\mathbf{b} \in V$ and $\mathbf{V}^T\mathbf{W}$ is nonsingular, then Test 1 is satisfied with $\varepsilon = \sqrt{m} \|\mathbf{A}\| \left\| (\mathbf{V}^T\mathbf{W})^{-1} \right\| \delta$.

Proof: Let $\mathbf{w}_i = \mathbf{A}\mathbf{v}_i$. Given $\left\| \mathbf{w}_i - \sum_{j=1}^m \langle \mathbf{w}_i, \mathbf{v}_j \rangle \mathbf{v}_j \right\| = \|\eta_i\| \leq \|\mathbf{A}\| \delta$. Consider,

$$\begin{aligned} \mathbf{b} - \sum_{i=1}^m \beta_i \mathbf{w}_i &= \mathbf{b} - \sum_{i=1}^m \beta_i \sum_{j=1}^m \langle \mathbf{w}_i, \mathbf{v}_j \rangle \mathbf{v}_j - \sum_{i=1}^m \beta_i \eta_i \\ &= \mathbf{b} - \sum_{j=1}^m \left(\sum_{i=1}^m \beta_i \langle \mathbf{w}_i, \mathbf{v}_j \rangle \right) \mathbf{v}_j - \sum_{i=1}^m \beta_i \eta_i \\ &= - \sum_{i=1}^m \beta_i \eta_i, \end{aligned}$$

if we choose $\sum_{j=1}^m \beta_i \langle \mathbf{w}_i, \mathbf{v}_j \rangle = \langle \mathbf{b}, \mathbf{v}_j \rangle$. This requires the solution of $(\mathbf{V}^T\mathbf{W})\beta = \mathbf{V}^T\mathbf{b}$, which in turn, requires that $\mathbf{V}^T\mathbf{W}$ be nonsingular. Hence,

$$\begin{aligned} \frac{\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\|}{\|\mathbf{b}\|} &\leq \frac{\|\mathbf{b} - \sum_{i=1}^m \beta_i \mathbf{w}_i\|}{\|\mathbf{b}\|} \\ &\leq \frac{\sum_{i=1}^m |\beta_i| \|\mathbf{A}\| \delta}{\|\mathbf{b}\|} \\ &= \frac{\|\beta\|_1 \|\mathbf{A}\| \delta}{\|\mathbf{b}\|} \\ &\leq \frac{\sqrt{m} \|\beta\|_2 \|\mathbf{A}\| \delta}{\|\mathbf{b}\|} \\ &\leq \|\mathbf{A}\| \left\| (\mathbf{V}^T\mathbf{W})^{-1} \right\| \sqrt{m} \delta, \end{aligned}$$

using $\beta = (\mathbf{V}^T\mathbf{W})^{-1} \mathbf{V}^T\mathbf{b}$ and $\|\mathbf{V}\|_2 = 1$ ($\mathbf{V}^T\mathbf{V} = \mathbf{I}$).



Notes:

- To see that $\mathbf{V}^T \mathbf{W}$ is nonsingular in most cases that arise, consider $\mathbf{V}^T \mathbf{W} \mathbf{c} = \mathbf{0}$. Either $\mathbf{W} \mathbf{c} = \mathbf{0}$ or $\mathbf{w} = \mathbf{W} \mathbf{c} \perp V$. The former is impossible, since \mathbf{W} has linearly independent columns. For latter,

$$1 = \frac{\|\mathbf{w} - \mathbf{0}\|}{\|\mathbf{w}\|} = \frac{\|\mathbf{w} - \mathcal{P}_V(\mathbf{w})\|}{\|\mathbf{w}\|} < \delta,$$

which is not possible. A possible problem does arise, however, if one of the \mathbf{v}_i is orthogonal to W .

- If \mathbf{A} is symmetric, then

$$\begin{aligned} \mu_0 &= \min_{\mathbf{y}} \frac{\mathbf{y}^T \mathbf{V}^T \mathbf{A} \mathbf{V} \mathbf{y}}{\mathbf{y}^T \mathbf{y}} \leq \frac{\beta^T \mathbf{V}^T \mathbf{A} \mathbf{V} \beta}{\beta^T \beta} = \frac{\beta^T \mathbf{V}^T \mathbf{b}}{\|\beta\|^2} \\ &= \frac{(\mathbf{V} \beta)^T \mathbf{b}}{\|\beta\|^2} \leq \frac{\|\mathbf{V} \beta\| \|\mathbf{b}\|}{\|\beta\|^2} \leq \frac{\|\mathbf{b}\|}{\|\beta\|} \end{aligned}$$

and therefore, $\|\beta\|/\|\mathbf{b}\| \leq 1/\mu_0$, that is

$$\frac{\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\|}{\|\mathbf{b}\|} \leq \frac{\|\mathbf{A}\| \sqrt{m}}{\mu_0} \delta,$$

where μ_0 is the minimum Ritz value of \mathbf{A} on V .

Theorem 6 *If (θ, \mathbf{x}) is a Ritz pair of \mathbf{A} with $\|\mathbf{x}\| = 1$ on an approximately invariant subspace V of order ε , then $\|\mathbf{A} \mathbf{x} - \theta \mathbf{x}\| \leq \|\mathbf{A}\| \varepsilon$.*

Proof: Since $\mathbf{x} = \mathbf{V} \mathbf{y}$, $\mathbf{A} \mathbf{x} = \mathbf{A} \mathbf{V} \mathbf{y} = (\mathbf{V} \mathbf{M} + \mathbf{S}) \mathbf{y} = \theta \mathbf{V} \mathbf{y} + \mathbf{S} \mathbf{y}$, where $\mathbf{V}^T \mathbf{S} = \mathbf{0}$ and $\mathbf{M} \mathbf{y} = \theta \mathbf{y}$ (by Lemma 4). Thus,

$$\|\mathbf{A} \mathbf{x} - \theta \mathbf{x}\| = \|\mathbf{S} \mathbf{y}\| \leq \|\mathbf{S}\| \|\mathbf{y}\| \leq \varepsilon \|\mathbf{A}\|, \text{ taking } \|\mathbf{x}\| = \|\mathbf{y}\| = 1.$$



5.1 Potential inaccuracies in the theoretical bounds

Consider the solution of the problem $\mathbf{Ax} = \mathbf{b}$ by the methodology described in Section 2. The residual

$$\begin{aligned} & \|\mathbf{b} - \mathbf{Ax}\| \\ = & \|\mathbf{b} - \mathcal{P}_W(\mathbf{b}) + \mathcal{P}_W(\mathbf{b}) - \mathcal{P}_W(\mathbf{Ax}) + \mathcal{P}_W(\mathbf{Ax}) - \mathbf{Ax}\| \\ \leq & \|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\| + \|\mathcal{P}_W(\mathbf{b}) - \mathcal{P}_W(\mathbf{Ax})\| + \|\mathcal{P}_W(\mathbf{Ax}) - \mathbf{Ax}\| \end{aligned}$$

consists of three terms. The first term expresses how well \mathbf{b} is captured in W . The second term gives the error in solving the problem on the low dimensional subspace, that is, the *exact reduced problem* which theoretically should be zero but depends on the errors due to the method employed and inexact floating point arithmetic. The third term expresses how well W captures the image of V . If one chooses W such that $\mathbf{b} \in W$ then the first term is zero and the error comes from the third term. To minimise the error $W = \mathbf{A}(V)$ is chosen so that the last term is zero and then choose V to be approximately invariant so that the first term will be reasonably small. These issues will be addressed rigorously in future research work to be undertaken by the authors.

6 Case studies

Much of the numerical analysis of large sparse matrices derives from the study of Krylov subspaces. In this section we consider the possibility that such spaces are approximately invariant. To test this proposition, two case studies are exhibited. The test matrices analysed were generated from the discretisation of three-dimensional

partial differential equations

$$\nabla \cdot (\mathbf{K} \nabla \varphi) = \gamma, \quad \mathbf{K} = \begin{pmatrix} a(\mathbf{x}) & 0 & 0 \\ 0 & b(\mathbf{x}) & 0 \\ 0 & 0 & c(\mathbf{x}) \end{pmatrix}. \quad (4)$$

A cube shaped region was used for the computational domain and the Dirichlet condition $\varphi = 0$ was adopted at the boundary. Since only the discretisation matrix is of importance for the analysis performed here, the right-hand side function γ was not considered. Note that in the two cases discussed throughout this section, classical finite volume strategies were used to derive the discrete analogues of (4) and all of the developed algorithms were implemented in MATLAB version 6 running under the Windows NT environment. The right hand side vector \mathbf{b} was taken as a random vector, with entries chosen from a normal distribution with mean zero, variance one and standard deviation one.

The following bases were examined for the detection of an approximately invariant subspace according to Lemma 3:

- *Krylov Basis* with Modified Gram-Schmidt Process used to generate the standard *ON* basis for $V = \mathcal{K}_\ell(\mathbf{b}, \mathbf{A})$:

$$\mathbf{U} = [\mathbf{b}, \mathbf{A}\mathbf{b}, \dots, \mathbf{A}^{\ell-1}\mathbf{b}] \equiv \mathbf{QR},$$

which is unstable but convergent (in direction) sequence.

- *Arnoldi Method* used to Generate *ON* basis for $V = \mathcal{K}_\ell(\mathbf{b}, \mathbf{A})$:

$$\mathbf{A}\mathbf{Q}_\ell = \mathbf{Q}_{\ell+1}\bar{\mathbf{H}}_\ell,$$

which is stable but does not produce a convergent sequence, where $\bar{\mathbf{H}}_\ell$ is an upper Hessenberg matrix with its elements defined by the Arnoldi algorithm.

If the Krylov subspace is going to be approximately invariant then any basis for it must satisfy the condition of Lemma 3 with sufficiently small δ .

6.1 Isotropic model

In this case study the parameters in (4) were set to $a(x, y, z) = b(x, y, z) = c(x, y, z) = 1$. The dimensions of the system were $n_x = n_y = n_z = 8$ which generated a total of 512 unknowns.

The initial approximation $\mathbf{x}_0 = (0, 0, \dots, 0)^T$ was used in GMRES. The norms of the system were $\|\mathbf{A}\|_1 = 12$, $\|\mathbf{A}\|_\infty = 12$, $\|\mathbf{A}\|_2 = 11.6382$ and $\|\mathbf{b}\|_2 = 13.1135$, the condition number of the coefficient matrix was $k_2(\mathbf{A}) = 32.1634$. The spectrum of eigenvalues ranged between $\lambda_{\min} = -11.6382$ and $\lambda_{\max} = -0.36184$. The parameter $\delta = 1 \times 10^{-25}$ in Lemma 3 enabled the approximately invariant subspace to be detected with dimension $\ell = 40$ and the norm of the solution residual computed from GMRES was $\|\mathbf{r}\|_2 = 1.16862 \times 10^{-10}$.

Figure 2(a) shows the reduction in the solution residual with increasing subspace dimension ℓ , while Figure 2(b) depicts the variation in $\sin \theta_\ell$ versus ℓ , where $\sin \theta_\ell$ refers to the test in Lemma 3 using the last basis vector in the approximate invariant subspace since the other basis vectors in the subspace theoretically already satisfy the condition. Observe from Figure 2(b) that the Arnoldi basis produces a pronounced oscillatory behaviour in $\sin \theta_\ell$. This behaviour indicates that it is unlikely the Krylov subspace is approximately invariant. However, the monotonically decreasing behaviour of the graph for the Krylov basis leads us to believe that the Krylov subspace could be in fact an approximately invariant subspace.

The order of the approximately invariant subspace was $\varepsilon =$

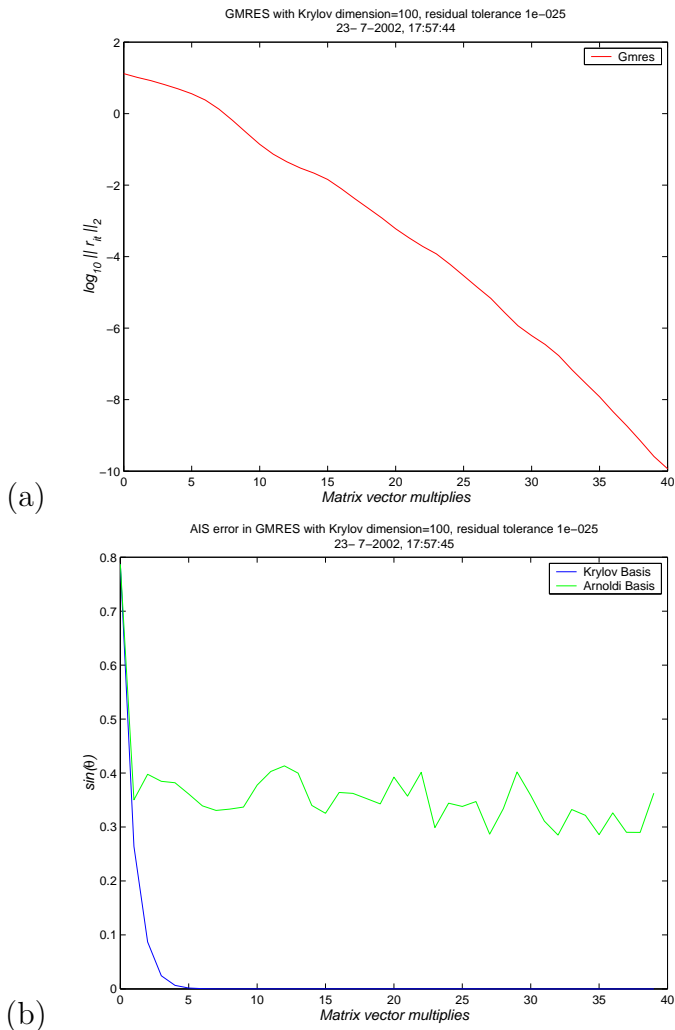


FIGURE 2: Results for the isotropic case study: (a) Reduction in the residual for GMRES; (b) The performance of Lemma 3 on detecting the approximately invariant subspace

$\|\mathbf{A}\|\delta/\mu_0 = 7.12642 \times 10^{-10}$, with $\mu_0 = 1.6331 \times 10^{-15}$. The error bound in this case was satisfied successfully as

$$\frac{\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\|}{\|\mathbf{b}\|} \equiv 8.9 \times 10^{-12} \leq \|\mathbf{A}\| \left\| (\mathbf{V}^T \mathbf{W})^{-1} \right\| \sqrt{\ell} \varepsilon \equiv 1.4 \times 10^{-7};$$

however, the bound in Lemma 4 could not be satisfied:

$$\|\mathbf{A}\mathbf{V} - \mathbf{V}\mathbf{B}\|_2 = 2.3 \not\leq \|\mathbf{A}\|_2 \varepsilon = 8.3 \times 10^{-9}.$$

6.2 Anisotropic model

The situation was almost exactly the same as stated above for the isotropic model. However, the functions $a(x, y, z) = 1$, $b(x, y, z) = 10$, $c(x, y, z) = 1000$ were used. The norms of the system in this case were computed as $\|\mathbf{A}\|_1 = 4044$, $\|\mathbf{A}\|_\infty = 4044$, $\|\mathbf{A}\|_2 = 3922.1$ and $\|\mathbf{b}\|_2 = 13.1135$ and the condition number $k_2(\mathbf{A}) = 32.1634$. The spectrum of eigenvalues ranged between $\lambda_{\min} = -3922.1$ and $\lambda_{\max} = -121.94$.

The statistics of the test are exhibited in Figure 3(a) for the reduction in the solution residual and Figure 3(b) for the variation in $\sin \theta_\ell$ with increasing subspace dimension ℓ . The oscillatory behaviour in $\sin \theta_\ell$ is again evident in Figure 3(b) for the Arnoldi basis, and again the monotonically decreasing behaviour of the graph for the Krylov basis leads us to believe that the Krylov subspace could be in fact an approximately invariant subspace.

In this case the parameter $\delta = 1 \times 10^{-25}$ in Lemma 3 enabled the approximately invariant subspace to be detected with dimension $\ell = 37$ and the norm of the solution residual computed from GMRES was $\|\mathbf{r}\|_2 = 1.1587 \times 10^{-7}$. The order of the approximately

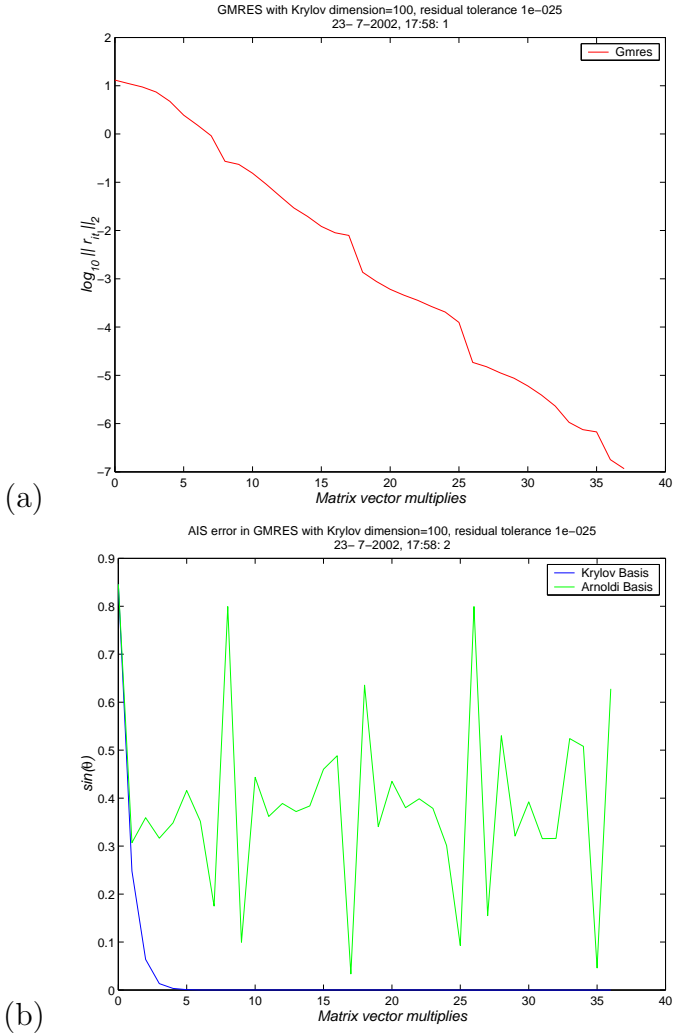


FIGURE 3: Results for the Anisotropic Case Study: (a) Reduction in the residual for GMRES; (b) The performance of Lemma 3 on detecting the approximately invariant subspace

invariant subspace was $\varepsilon = \|\mathbf{A}\|\delta/\mu_0 = 7.69094 \times 10^{-10}$, with $\mu_0 = 5.09958 \times 10^{-13}$. The error bound in this case was satisfied successfully as

$$\frac{\|\mathbf{b} - \mathcal{P}_W(\mathbf{b})\|}{\|\mathbf{b}\|} \equiv 8.8 \times 10^{-9} \leq \|\mathbf{A}\| \left\| (\mathbf{V}^T \mathbf{W})^{-1} \right\| \sqrt{\ell} \varepsilon \equiv 1.5 \times 10^{-7}.$$

Again the bound in Lemma 4 could not be satisfied:

$$\|\mathbf{A}\mathbf{V} - \mathbf{V}\mathbf{B}\|_2 = 1317 \not\leq \|\mathbf{A}\|_2 \varepsilon = 3.0 \times 10^{-6}.$$

The results presented above for both case studies definitely warrant further investigations. If there are problems in our results it is suspected that the source of the error seems to arise from the magnitude of μ_0 which appears to be of the same order as δ . Furthermore, the algorithm used for computing μ_0 in MATLAB may not provide sufficient accuracy for the computations.

7 Conclusions

In this paper a new definition of an approximately invariant subspace was introduced that could be useful for solving large-scale linear systems or the algebraic eigenvalue problem. The sensitivity of the basis used for detecting when a subspace is approximately invariant was elucidated and, using the definition, theoretical error bounds were placed on the two standard numerical linear algebra problems, which will be the subject of further investigations. Future work also must consider how these theoretical results transfer to floating point computations. The primary objective of this work was to lay solid theoretical foundations that could pave the way for developing a new solution strategy to overcome the problems associated with Krylov methods discussed in the introduction. Krylov

subspace methods seek to construct an approximately invariant subspace of low dimension that contains \mathbf{b} and hopefully the solution \mathbf{x} of $\mathbf{Ax} = \mathbf{b}$. A more direct approach might be to construct an invariant subspace of low dimension that contains the solution \mathbf{x} . The theory proposed here can enable this possibility to be examined rigorously in future research.

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References

- [1] Y. Saad and M. H. Schultz (1986), GMRES: a generalized minimum residual algorithm for solving nonsymmetric linear systems, *SIAM J. Scientific and Statistical Computing*, 7, pp.856–869. [C380](#)
- [2] Y. Saad (1996), *Iterative Methods for Sparse Linear Systems*, PWS publishing Company, ITS. [C380](#), [C381](#)
- [3] I. C. F. Ipsen and C. D. Meyer, (1998) *The Idea Behind Krylov Methods*, Report, Department of Mathematics, North Carolina State University, Raleigh, NC 27695-8205, USA [C380](#), [C384](#)
- [4] C. C. Paige and M. A. Saunders (1975), Solution of sparse indefinite systems of linear equations, *SIAM J. Numerical Analysis*, 12, pp.617–629. [C380](#)
- [5] G. W. Stewart, (1998), *Afternotes goes to Graduate School*, Lectures on Advanced Numerical Analysis, SIAM. [C380](#), [C388](#)