

Note on Krylov subspace methods^{*}

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[1] Higham, N. J. (2023). Numerical linear algebra and matrix analysis. Unpublished manuscript.

1 Introduction

The k th Krylov subspace of $A \in \mathbb{C}^{n \times n}$ and a nonzero vector $b \in \mathbb{C}^n$ is defined by

$$\mathcal{K}_k(A, b) = \text{span}\{b, Ab, \dots, A^{k-1}b\}.$$

In the Krylov subspace method for solving a linear system $Ax = b$, each iterate x_k is chosen from the shifted Krylov subspace $x_0 + \mathcal{K}_k(A, r_0)$, where $r_0 = b - Ax_0$, that is,

$$x_k - x_0 \in \mathcal{K}_k(A, r_0). \quad (1.1)$$

We can rewrite (1.1) as

$$x_k - x_0 = \sum_{i=0}^{k-1} \alpha_i A^i r_0 =: q_{k-1}(A)r_0,$$

where q_{k-1} is a polynomial of degree at most $k-1$. Multiply by A gives,

$$Ax_k - Ax_0 = Aq_{k-1}(A)r_0,$$

using the definition $r_k := b - Ax_k$, we have

$$r_k - r_0 = Aq_{k-1}(A)r_0$$

or

$$r_k = q_k(A)r_0,$$

where p_k is a polynomial of degree at most k with $q_k(0) = 1$. The minimal residual method (MINRES) for symmetric matrix, and the generalized minimal residual method (GMRES) for general A . In both cases, $x_k \in x_0 + \mathcal{K}_k(A, r_0)$ to minimize $\|r_k\|_2^2$.

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2 The Arnoldi Method

The Arnoldi process for $A \in \mathbb{C}^{n \times n}$ attempts to compute the Hessenberg reduction $Q^*AQ = H$, where $Q \in \mathbb{C}^{n \times n}$ is unitary and $H \in \mathbb{C}^{n \times n}$ is upper Hessenberg. Write $Q = [q_1, \dots, q_n]$ and equating k th columns in $AQ = QH$ gives

$$Aq_k = \sum_{i=1}^{k+1} h_{ik}q_i, \quad k = 1 : n-1, \quad (2.1)$$

and for the n th column we have

$$Aq_n = \sum_{i=1}^n h_{in}q_i.$$

(2.1) may also be rewritten as

$$h_{k+1,k}q_{k+1} = Aq_k - \sum_{i=1}^k h_{ik}q_i, \quad k = 1 : n-1. \quad (2.2)$$

Using the fact that the columns of Q are orthonormal. By choosing an arbitrary $j = 1 : k$, we have

$$q_j^*q_{k+1}h_{k+1,k} = q_j^*Aq_k - \sum_{i=1}^k h_{ik}q_j^*q_i.$$

Notice that the latter term is only nonzero if i is taken to be the same value as j . Therefore, by choosing $i = j$, we have

$$0 = q_j^*Aq_k - h_{jk} \Rightarrow h_{jk} = q_j^*Aq_k, \quad j = 1 : k.$$

Let us define $r_k := Aq_k - \sum_{i=1}^k h_{ik}q_i$, the right hand side of (2.2). Then we can write it as $h_{k+1,k}q_{k+1} = r_k$. If $r_k \neq 0$, then $q_{k+1} = r_k/h_{k+1,k}$, with $h_{k+1,k} = \|r_k\|_2$. If $r_k = 0$, the process will terminate within. Notice that, we have already obtain the algorithm implicitly. Here, r_k can be computed prior to q_k , and the algorithm can proceed.

To illustrate the difference between the combined version and separate version as discussed in Algorithm 1, we provide a small numerical experiment. Figure 1 shows the backward error and the orthogonality error. We observe that using the combined version, both error are significantly smaller than the separate one.

From (2.2), it follows by induction that

$$\text{span}\{q_1, \dots, q_k\} = \text{span}\{q_1, Aq_1, \dots, Aq_{k-1}\},$$

that is, the Arnoldi vectors $\{q_i\}_{i=1}^k$ form an orthonormal basis for the Krylov subspace $\mathcal{K}_k(A, q_1)$.

The eigenvalues of the Hessenberg matrix H_m produced by the Arnoldi process are called **Ritz values** and the corresponding eigenvectors are **Ritz vectors**. If (λ, v) is an eigenpair of H_k , then (λ, Q_kv) is an approximate eigenpair of A .

After k stages, the Arnoldi process produces the factorization

$$AQ_k = Q_kH_k + h_{k+1,k}q_{k+1}e_k^T, \quad (2.3)$$

Algorithm 1. *Arnoldi process with modified Gram-Schmidt orthogonalization.*

Input: Given a square matrix $A \in \mathbb{C}^{n \times n}$, a starting vector q_1 with unit 2 norm.

Output: A column-wise orthonormal matrix $Q \in \mathbb{C}^{n \times m}$ and a upper Hessenberg matrix $H \in \mathbb{C}^{m \times m}$, such that $A = QHQ^*$.

```
1: for  $k = 1 : n$  do                                     % For  $k = n$ , the only part that will be executed is
   the generation of the  $n$ th column of  $H$ . Afterwards, the 2-norm of " $h_{n+1,n}$ " will definitely
   becomes zero since there are only  $n$  basis for a  $n$  dimensional vector space.
2:    $w_k = Aq_k$ 
3:   for  $j = 1 : k$  do
4:      $h_{jk} = q_j^* w_k$ 
5:      $w_k = w_k - h_{jk} q_j$ 
6:   end for                                             % When we started
   from  $w_k = Aq_k$ , we generated the "temporary"  $(k+1)$ th basis. In order to make the newly
   generated basis orthogonal to  $q_1, \dots, q_k$ , we need to delete the corresponding components,
   as described in (2.1) and (2.2). However, the question is the definition of  $h_{jk}$  is  $q_j^* Aq_k$ , but
   how can we keep "modify"  $Aq_k$ ,  $w_k$ ? The answer can be seen from (2.1). After the first
   iteration, we get  $w_k = \sum_{i=2}^{k+1} h_{ik} q_i$ . In the second iteration, when pre-multiply  $q_2^*$  to  $w_k$ ,
   we will not getting any contribution from  $h_{1k} q_1$ , even though in the scenario we do not remove
   it, since  $q_1$  and  $q_2$  are constructed to be orthonormal. Therefore
```

$$q_2^* \sum_{i=1}^{k+1} h_{ik} q_i = q_2^* \sum_{i=2}^{k+1} h_{ik} q_i.$$

Therefore, removing the computed component is mathematically equivalent to the un-removed version. The next question is *why we doing in this removing approach*. Firstly, one should notice that if we do these two steps in the loop separately like:

```
for  $j = 1 : k$  do  $h_{jk} = q_j^* w_k$  end for
for  $j = 1 : k$  do  $w_k = w_k - h_{jk} q_j$  end for
```

This is mathematically equivalent to the combined one. This approach is purely for numerical consideration. Since in floating point arithmetic, the inner product of two orthonormal vectors may not be zero but a small number about u , the unit roundoff. Therefore, without removing the previous parts, it is possible that, at the k th step, all the vectors q_1, \dots, q_{k-1} will contaminate the entries of H , which leads to an inaccurate decomposition.

```
7:   if  $\|w_k\|_2 = 0$  then
8:     quit
9:   else
10:     $h_{k+1,k} = \|w_k\|_2$ 
11:   end if
12:    $q_{k+1} = w_{k+1}/h_{k+1,k}$                                % Normalize the generated vector.
13: end for
```

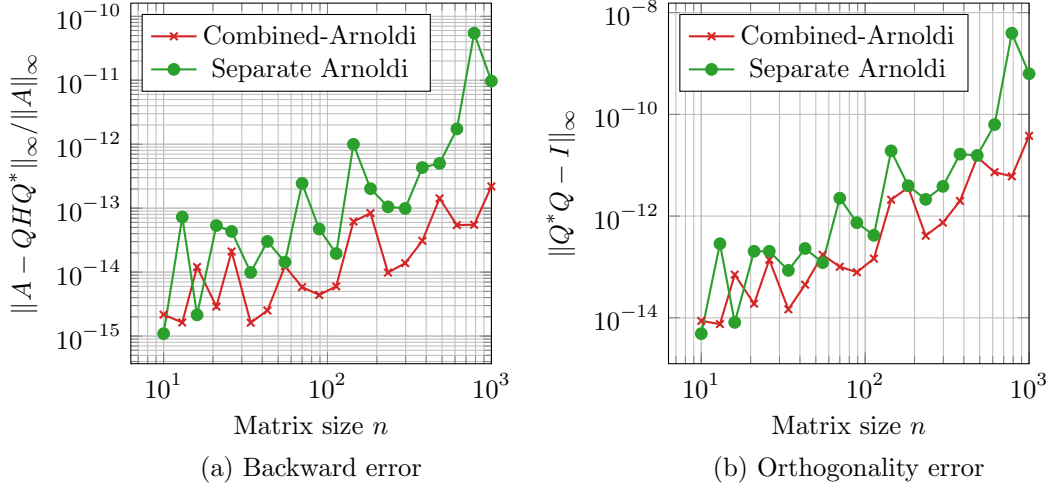


Figure 1: Behavior of the backward error and the orthogonality error for computed Hessenberg reduction using combined and separate version of Algorithm 1. The test matrix is generated with `randn(n)`.

where $Q_k = [q_1, \dots, q_k]$ and $H_k = (h_{ij})$ is $k \times k$ upper Hessenberg. From (2.3), we have

$$AQ_k v = Q_k H_k v + h_{k+1,k} q_{k+1} e_k^T v = \lambda Q_k v + h_{k+1,k} v_k q_{k+1},$$

where v_k is the k th entry of v , so that

$$\|(A - \lambda I)Q_k v\|_2 = |h_{k+1,k}| |v_k|. \quad (2.4)$$

Therefore, if one wants to test the convergence of the eigensolver, it is no need to form $Q_k v$. Only monitoring the subdiagonal elements of H and the last coordinate of its eigenvalue is sufficient.

If $h_{k+1,k} = 0$, then (2.4) implies $(\lambda, Q_k v)$ is an exact eigenpair of A . In this case, $AQ_k = Q_k H_k$ by (2.3), so the columns of Q_k span an invariant subspace of A , and all the eigenvalues of H are eigenvalues of A .

3 The Generalized Minimal Residual Method

Any vector x in the shifted Krylov subspace $x_0 + \mathcal{K}_k(A, r_0)$ can be written as $x = x_0 + Q_k y$ for some $y \in \mathbb{C}^k$, where columns of $Q_k \in \mathbb{C}^{n \times k}$ are a basis for $\mathcal{K}_k(A, r_0)$. The GMRES method minimizes

$$r = b - Ax = b - Ax_0 - AQ_k y = r_0 - AQ_k y \quad (3.1)$$

over all y . In order to do so, it needs to build the matrix Q_k using the Arnoldi process (Algorithm 1).

Suppose we run the Arnoldi process with $q_1 = r_0 / \beta$, where $\beta = \|r_0\|_2$. We can rewrite (2.3) as

$$AQ_k = Q_k \tilde{H}_k, \quad \tilde{H}_k = \begin{bmatrix} H_k \\ h_{k+1,k} e_k^T \end{bmatrix} \quad (3.2)$$

Then using (3.1) and (3.2), we have

$$r = r_0 - AQ_k y \quad (3.3)$$

$$\begin{aligned} &= r_0 - Q_{k+1} \tilde{H}_k y \\ &= \beta q_1 - Q_{k+1} \tilde{H}_k y \\ &= Q_{k+1} (\beta e_1 - \tilde{H}_k y) \end{aligned} \quad (3.4)$$

and hence

$$\|r\|_2 = \|\beta e_1 - \tilde{H}_k y\|_2,$$

since Q_{k+1} has orthonormal columns. Then minimizing r over all y reduces to a least square problem with an $(m+1) \times m$ Hessenberg coefficient matrix, which can be solved by Givens QR factorization in $O(m^2)$ flops. **The GMRES method combines the Arnoldi process with solution of the least square problem (3.4).**

Algorithm 2. *GMRES - Arnoldi process with least square solution*

Input: $A \in \mathbb{C}^{n \times n}$, $b \in \mathbb{C}^n$ and a starting vector $x_0 \in \mathbb{C}^n$.

Output: A solution $x \in \mathbb{C}^n$ that solves the linear system $Ax = b$.

```

1:  $m = n$ ,  $r_0 = b - Ax_0$ ,  $\beta = \|r_0\|_2$ ,  $q_1 = r_0/\beta$ 
2: for  $k = 1 : m$  do
3:    $w_k = Aq_k$ 
4:   for  $i = 1 : k$  do
5:      $h_{i,k} = q_i^* w_k$ 
6:      $w_k = w_k - h_{ik} q_i$ 
7:   end for
8:    $h_{k+1,k} = \|w_k\|_2$ 
9:   if  $h_{k+1,k} = 0$  then
10:    Set  $m = k$  and quit the loop
11:   end if
12:    $q_{k+1} = w_k / h_{k+1,k}$ 
13: end for
```

Until now, this is simply Algorithm 1, the Arnoldi process for constructing a Hessenberg reduction. Now, we have $AQ_k = Q_k \tilde{H}_k$ as shown in (3.2).

14: Compute the solution y_m for the least square problem $\min_{y_m} \|\beta e_1 - \tilde{H}_m y_m\|_2$. Here, we set $\tilde{H}_m = H_m$ if $h_{m+1,m} = 0$.

15: Recover the solution via $x = x_0 + Q_{m+1} y_m$ or $x = x_0 + Q_m y_m$ if $h_{m+1,m} = 0$.

GMRES requires $O(mn^2)$ flops for a full matrix (the dominant cost is the matrix-vector product on Line 3) and $O(mn)$ elements of storage for Q_m . If m is large, the computation and storage costs are both prohibitive. Therefore, it is common to terminate the algorithm prematurely and restart it: the iteration stops after $p \ll n$ iterations and reruns using the current approximation x_p as a new starting vector x_0 . The method with restarts after every k iterations is denoted by **GMRES(k)**.

References

- [1] Nicholas J. Higham. Numerical linear algebra and matrix analysis. Unfinished book (Version 2023 June 23), 2023. (Cited on p. 1)