



Computation of matrix functions with deflated restarting[☆]

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ARTICLE INFO

Article history:

Received 28 December 2010

Received in revised form 5 March 2012

Keywords:

Matrix functions

Krylov subspace approximation

Restarted Arnoldi method

Deflated restarting Krylov subspace method

ABSTRACT

A deflated restarting Krylov subspace method for approximating a function of a matrix times a vector is proposed. In contrast to other Krylov subspace methods, the performance of the method in this paper is better. We further show that the deflating algorithm inherits the superlinear convergence property of its unrestarted counterpart for the entire function and present the results of numerical experiments.

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1. Introduction

The evaluation of

$$f(A)v \tag{1.1}$$

where $A \in \mathbb{C}^{n \times n}$, $v \in \mathbb{C}^n$ and $f: \mathbb{C} \supset D \rightarrow \mathbb{C}$ is a function for which $f(A)$ is defined, is a common computational task. One of the most important applications in which (1.1) appears is the solution of ordinary differential equations [1,2] or of time-dependent partial differential equations [3,4]. There are several other cases in which the computation of (1.1) is required, such as identification problems for semigroups involving the logarithm [5], lattice quantum chromodynamics simulations requiring the evaluation of the matrix sign function [6].

In many of the applications mentioned above the matrix A is large and sparse or structured. In this case evaluating (1.1) by first forming $f(A)$ and then multiplying with v is usually unfeasible. Here Krylov subspace approximation of (1.1) is popular [1–35].

Let A be a complex square matrix of (large) dimension N , and a given vector $v \in \mathbb{C}^N$. Without loss of generality we also assume that $\|v\| = 1$ in this paper. The Arnoldi process generates an orthonormal basis $V_m = [v_1, v_2, \dots, v_m]$ of the Krylov space $K_m(A, v) = \text{Span}\{v, Av, \dots, A^{m-1}v\}$ and a Hessenberg matrix of dimension m (which is the upper left part of its successor H_m) such that

$$AV_m = V_m H_m + \eta_{m+1,m} v_{m+1} (e_m^{(m)})^T$$

which $e_m^{(i)}$ is the i th unit vector in $\mathbb{R}^m$. The Arnoldi approximation to $f(A)v$ is then defined by

$$f_m = V_m f(H_m) e_m^{(1)}. \tag{1.2}$$

This technique first appeared in the literature in the 1980s [32–35] and can now be viewed as standard. The advantage of this approach is that it requires A only for computing matrix–vector products and that, for smooth functions such as the

[☆] The work are supported by Shanghai Natural Science Foundation (10ZR1410900) and by Key Disciplines of Shanghai Municipality (S30104).

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exponential, it converges superlinearly [7–9]. One shortcoming of the approximation is that it requires that the complete basis of $K_m(A, v)$ be available, which can be prohibitive for large A and large values of m .

Reducing storage and computational requirements was the motivation behind the restarting algorithm proposed in [12]. Unfortunately, one has to take into account a slower convergence rate, since at each restart some information is discarded. Especially in the presence of small eigenvalues in the iteration matrix, the convergence rate of restart Krylov space may be worse than that of full Krylov space. To improve the convergence rate, we give the deflated restarting Krylov subspace method for computing matrix functions.

The paper is organized as follows. In Section 2, we review the general framework of the restarted Krylov space method for computing matrix functions. In Section 3 we introduce the deflated restarting Arnoldi process and steps using Arnoldi-like decomposition. We also give an efficient algorithm of the deflated restarting Arnoldi approximation for a matrix function. In Section 4, we give the convergence analysis of the deflated restarting Krylov subspace method. In Section 5, we demonstrate the performance of the deflated restarting method for several test problems.

2. The restarted Krylov subspace method for matrix functions

The restarted Krylov subspace algorithm proposed in [12] proceeds by repeatedly generating a basis of Krylov spaces of fixed dimension m , updating the most recent approximation to (1.1), and then discarding all but the last basis vector, which is subsequently used as the initial vector for the next Krylov space. The result of h cycles of this restarting scheme is the Krylov subspace approximation associated with decomposition

$$A\widehat{V}_m^{(h)} = \widehat{V}_m^{(h)}\widehat{H}_m^{(h)} + \eta_{h+1}v_{hm+1}(e_{hm}^{(hm)})^T, \quad (2.1)$$

where $\widehat{V}_m^{(h)} = [V_m^{(1)}, V_m^{(2)}, \dots, V_m^{(h)}] \in \mathbb{C}^{n \times hm}$,

$$\widehat{H}_m^{(h)} = \begin{bmatrix} H_m^{(1)} & & & & \\ E^{(2)} & H_m^{(2)} & & & \\ & \ddots & \ddots & & \\ & & E^{(h)} & H_m^{(h)} & \end{bmatrix}$$

and $E^{(j)} = \eta_j e_m^{(1)} (e_m^{(m)})^T \in \mathbb{R}^{m \times m}$, $j = 2, \dots, h$.

Setting

$$\widehat{F}^{(h)} = f(\widehat{H}_m^{(h)}) = \begin{bmatrix} F^{1,1} & & & \\ F^{2,1} & F^{2,2} & & \\ \vdots & \vdots & \ddots & \\ F^{h,1} & F^{h,2} & \dots & F^{h,h} \end{bmatrix},$$

where $F^{jj} = f(H_m^{(j)})$, $j = 1, 2, \dots, h$. The approximation after h restart cycles is given by

$$\begin{aligned} \widehat{f}^{(h)} &= \widehat{V}_m^{(h)} f(\widehat{H}_m^{(h)}) e_{hm}^{(1)} = [V_m^{(1)}, V_m^{(2)}, \dots, V_m^{(h)}] \widehat{F}^{(h)} e_{hm}^{(1)} \\ &= \widehat{f}^{(h-1)} + V_m^{(h)} F^{h,1} e_m^{(1)}. \end{aligned} \quad (2.2)$$

3. The deflated restarting Krylov subspace method for matrix functions

It is well known that the convergence of Krylov subspace methods for linear equations depends to a large degree on the distribution of eigenvalues. And if there are small eigenvalues, then removing or deflating them can greatly improve the convergence rate. Likewise, for the problem of computing an eigenvalue, deflating nearby eigenvalues is helpful. Some recent approaches deflate restarted Krylov methods. These are mentioned for both eigenvalues and linear equations [36]. The deflated restarting Krylov subspace method is shown as follows.

Algorithm 1. Deflated Restarting Krylov subspace method in [36].

Step 1. start: Choose m and k .

Step 2. first cycle: Apply Standard **Arnoldi(m)** iteration, generate V_{m+1} and $\bar{H}_m$, then $AV_m = V_{m+1}\bar{H}_m$.

Step 3. eigenvector computation: Compute the k smallest (or others, if desired) eigenpairs (θ_i, g_i) of H_m , the m by m portion of $\bar{H}_m$.

Step 4. orthonormalization of first k vectors: Orthonormalize g_i 's, in order to form an m by k matrix P_k .

Step 5. Set $V_k = V_m P_k$, $v_{k+1} = v_{m+1}$, $H_k = P_k^T H_m P_k$, $\bar{H}_k = \begin{bmatrix} H_k \\ \bar{H}(m+1, m)(e_m^{(m)})^T P_k \end{bmatrix}$, then $AV_k = V_{k+1}\bar{H}_k$.

Step 6. Arnoldi iteration: Apply the Arnoldi iteration from this point to form the rest of V_{m+1} and $\bar{H}_m$.

Step 7. restart: Go to 3.

Remark. In step 5, $\text{Span}\{v_1, v_2, \dots, v_k\} = \text{Span}\{y_1, y_2, \dots, y_k\}$, where y_i ($i = 1, 2, \dots, k$) is a Ritz vector. The column of V_{k+1} is orthogonal.

The focus of this paper is on computation of matrix function with deflated restarting. Therefore, now we begin to analyze the deflated restarting Arnoldi process and the steps using Arnoldi-like decomposition in the following.

After the first standard Arnoldi process,

$$AV_m^{(1)} = V_m^{(1)}H_m^{(1)} + \eta_2 v_{m+1}(e_m^{(m)})^T. \quad (3.1)$$

The following is the deflation Arnoldi process. From step 3 to step 5, we can obtain

$$AV_k^{(2)} = V_{k+1}^{(2)}\bar{H}_k^{(2)}$$

namely

$$AV_k^{(2)} = V_k^{(2)}H_k^{(2)} + \eta_2 v_{m+1}(e_m^{(m)})^T P_k^{(2)}. \quad (3.2)$$

From step 6 we have

$$AV_{m-k}^{(2)} = [V_k^{(2)}, V_{m-k}^{(2)}]H_{m-k}^{(2)} + \eta_3 v_{2m+1}(e_{m-k}^{(m-k)})^T. \quad (3.3)$$

We glued the decompositions (3.2) and (3.3) together

$$AV_m^{(2)} = V_m^{(2)}H_m^{(2)} + \eta_3 v_{2m+1}(e_m^{(m)})^T, \quad (3.4)$$

where

$$V_m^{(2)} = [V_k^{(2)}, V_{m-k}^{(2)}], \quad H_m^{(2)} = \begin{bmatrix} H_k^{(2)} & \\ \eta_2 e_{m-k}^{(1)}(e_m^{(m)})^T P_k^{(2)} & H_{m-k}^{(2)} \end{bmatrix}.$$

We note that the columns of $\hat{V}_m^{(2)} = [V_m^{(1)}, V_m^{(2)}]$ form a basis of $K_{2m}(A, v)$, albeit not an orthonormal one, and we may combine the two decompositions (3.1) and (3.4) to the Arnoldi-like decomposition

$$A\hat{V}_m^{(2)} = \hat{V}_m^{(2)}\hat{H}_m^{(2)} + \eta_3 v_{2m+1}(e_{2m}^{(2m)})^T, \quad (3.5)$$

where

$$\hat{V}_m^{(2)} = [V_m^{(1)}, V_m^{(2)}], \quad \hat{H}_m^{(2)} = \begin{bmatrix} H_m^{(1)} & & \\ 0 & H_k^{(2)} & \\ N^{(2)} & M^{(2)} & H_{m-k}^{(1)} \end{bmatrix},$$

$$N^{(2)} = \eta_2 e_{m-k}^{(1)}(e_m^{(m)})^T, \quad M^{(2)} = \eta_2 e_{m-k}^{(1)}(e_m^{(m)})^T P_k^{(2)}.$$

The Krylov subspace approximation is given by

$$\begin{aligned} \hat{f}^{(2)} &= \hat{V}_m^{(2)} f(\hat{H}_m^{(2)}) e_{2m}^{(1)} = V_m^{(1)} f(H_m^{(1)}) e_m^{(1)} + V_m^{(2)} F^{2,1} e_m^{(1)} \\ &= \hat{f}^{(1)} + [V_k^{(2)}, V_{m-k}^{(2)}] F^{2,1} e_m^{(1)}, \end{aligned}$$

$$\text{where } f(\hat{H}_m^{(2)}) = \begin{bmatrix} f(H_m^{(1)}) & 0 \\ F^{2,1} & f(H_{m-k}^{(2)}) \end{bmatrix}.$$

The result of h cycles of this restarting scheme is the Krylov subspace approximation associated with decomposition

$$A\hat{V}_m^{(h)} = \hat{V}_m^{(h)}\hat{H}_m^{(h)} + \eta_{h+1} v_{hm+1}(e_{hm}^{(hm)})^T,$$

where

$$\hat{V}_m^{(h)} = [V_m^{(1)}, V_k^{(2)}, V_{m-k}^{(2)}, \dots, V_k^{(h)}, V_{m-k}^{(h)}] \in \mathbb{C}^{n \times hm},$$

$$\hat{H}_m^{(h)} = \begin{bmatrix} H_m^{(1)} & & & & & \\ \boxed{\begin{matrix} 0 \\ N^{(2)} \end{matrix}} & \boxed{\begin{matrix} H_k^{(2)} & H_{m-k}^{(2)} \\ M^{(2)} & \end{matrix}} & & & & \\ & \boxed{\begin{matrix} 0 \\ N^{(3)} \end{matrix}} & \boxed{\begin{matrix} H_k^{(3)} & H_{m-k}^{(3)} \\ M^{(3)} & \end{matrix}} & & & \\ & & \ddots & \ddots & \ddots & \\ & & & \boxed{\begin{matrix} 0 \\ N^{(h)} \end{matrix}} & \boxed{\begin{matrix} H_k^{(h)} & H_{m-k}^{(h)} \\ M^{(h)} & \end{matrix}} \end{bmatrix},$$

$$N^{(j)} = \eta_j e_{m-k}^{(1)}(e_m^{(m)})^T \in \mathbb{C}^{(m-k) \times m},$$

$$M^{(j)} = \eta_j e_{m-k}^{(1)}(e_m^{(m)})^T P_k^{(j)} \in \mathbb{C}^{(m-k) \times k}, \quad j = 2, 3, \dots, h.$$

Setting

$$\widehat{F}^{(h)} = f(\widehat{H}_m^{(h)}) = \begin{bmatrix} F^{1,1} & & & \\ F^{2,1} & F^{2,2} & & \\ \vdots & \vdots & \ddots & \\ F^{k,1} & F^{k,2} & \dots & F^{h,h} \end{bmatrix},$$

where $F^{jj} = f(H_m^{(j)})$, $j = 1, 2, \dots, h$. The approximation after h restart cycles is given by

$$\begin{aligned} \widehat{f}^{(h)} &= \widehat{V}_m^{(h)} f(\widehat{H}_m^{(h)}) e_{hm}^{(1)} = [V_m^{(1)}, V_m^{(2)}, \dots, V_m^{(h)}] \widehat{F}^{(h)} e_{hm}^{(1)} \\ &= \widehat{f}^{(h-1)} + V_m^{(h)} F^{h,1} e_m^{(1)}. \end{aligned} \quad (3.6)$$

Now, the crucial issue is the fast and stable computation of the coefficient vector $F^{h,1} e_m^{(1)}$ to update the approximation (3.6). We consider the implementation, which is built on a standard algorithm such as MATLAB's *funm*. The resulting process is a new algorithm for the computation of $f(A)v$, which is summarized as follows.

Algorithm 2. Deflated Restarting Arnoldi approximation for $f(A)v$.

Given: A, v, f

Choose m and k

Compute standard Arnoldi decomposition

$$AV_m^{(1)} = V_m^{(1)} H_m^{(1)} + \eta_2 v_{m+1} (e_m^{(m)})^T$$

$$f^{(1)} = V_m^{(1)} f(H_m^{(1)}) e_m^{(1)}$$

For $h = 2, 3, \dots$ **until convergence do**

 Compute the Arnoldi-like decomposition

$$A[V_k^{(h)}, V_{m-k}^{(h)}] = [V_k^{(h)}, V_{m-k}^{(h)}] \begin{bmatrix} H_k^{(h)} & H_{m-k}^{(h)} \\ M^{(h)} & \end{bmatrix} + \eta_{h+1} v_{hm+1} (e_m^{(m)})^T$$

$$\widehat{H}_m^{(h)} = \begin{bmatrix} \widehat{H}_m^{(h-1)} & & \\ 0 & H_k^{(h)} & \\ \eta_h e_{m-k}^{(1)} (e_{(h-1)m}^{(1)})^T & M^{(h)} & H_{m-k}^{(h)} \end{bmatrix}$$

 Update the approximation

$$\widehat{f}^{(h)} = \widehat{f}^{(h-1)} + V_m^{(h)} [f(\widehat{H}_m^{(h)}) e_m^{(1)}]_{(h-1)m+1:hm}$$

4. Convergence

For sufficiently smooth functions, restarting the Arnoldi approximation preserves its superlinear convergence, as shown in [12]. In this section, we show that the deflated restarting Arnoldi approximation still preserves the same convergence property. We state the following result for entire functions of order one (cf. [37, Section 2.1]), a class which includes the exponential function, and note that the result generalizes to other orders with minor modifications.

Theorem 1. Given $A \in \mathbb{C}$ and an entire function f of order one, let $\widehat{f}^{(h)}$ ($h \geq 2$) denote the deflated restarting Krylov subspace approximation after h restart cycles. Then there exist constants C and γ which are independent of m such that

$$\|f(A)v - \widehat{f}^{(h)}\| \leq C \frac{\gamma^{m-1}}{(m-1)!} \quad \text{for all } m.$$

Proof. After the first standard Arnoldi process

$$AV_m^{(1)} = V_m^{(1)} H_m^{(1)} + \eta_2 v_{m+1} (e_m^{(m)})^T.$$

The error expression is given as follows.

$$E_1 = f(A)v - V_m^{(1)} f(H_m^{(1)}) e_m^{(1)}.$$

Here, the Krylov subspace approximation $\widehat{f}^{(1)} = V_m^{(1)} f(H_m^{(1)}) e_m^{(1)} = p_{m-1}^{(1)}(A)v$, where $p_{m-1}^{(1)} \in \mathcal{P}_{m-1}$ denotes the polynomial of degree at most $m-1$, which interpolates f in the Hermite sense at the eigenvalues of $H_m^{(1)}$, i.e., at the Ritz values of A with respect to $K_m(A, v)$. Therefore

$$E_1 = f(A)v - V_m^{(1)} f(H_m^{(1)}) e_m^{(1)} = (f(A) - p_{m-1}^{(1)}(A))v. \quad (4.1)$$

We note that the error (4.1) is still a function of a matrix times a vector, so the approximation of the following deflation Arnoldi process is regarded as a correction for the previous error term.

After the first deflation Arnoldi process

$$AV_m^{(2)} = V_m^{(2)}H_m^{(2)} + \eta_3 v_{2m+1}(e_m^{(m)})^T,$$

$$\text{where } V_m^{(2)} = [V_k^{(2)}, V_{m-k}^{(2)}], H_m^{(2)} = \begin{bmatrix} H_k^{(2)} \\ \eta_2 e_{m-k}^{(1)}(e_m^{(m)})^T p_k^{(2)} H_{m-k}^{(2)} \end{bmatrix}.$$

The error expression is given in the following

$$E_2 = (f(A) - p_{m-1}^{(1)}(A))v - V_m^{(2)}(f(H_m^{(2)}) - p_{m-1}^{(1)}(H_m^{(2)}))e_m^{(1)}.$$

Here, the Krylov subspace approximation $\hat{f}^{(2)} = V_m^{(2)}(f(H_m^{(2)}) - p_{m-1}^{(1)}(H_m^{(2)}))e_m^{(1)} = p_{m-1}^{(2)}(A)v$, where $p_{m-1}^{(2)} \in \mathcal{P}_{m-1}$, which interpolates $f - p_{m-1}^{(1)}$ in the Hermite sense at the eigenvalues of $H_m^{(2)}$, i.e., at the Ritz values of A with respect to $K_m(A, V_m^{(2)}(\cdot, 1))$. Therefore

$$E_2 = (f(A) - p_{m-1}^{(1)}(A) - p_{m-1}^{(2)}(A))v. \quad (4.2)$$

After $h - 1$ restart cycles, the error expression is given in the following.

$$E_{h-1} = (f(A) - p_{m-1}(A))v, \quad (4.3)$$

where $p_{m-1}(A) = p_{m-1}^{(1)}(A) + p_{m-1}^{(2)}(A) + \dots + p_{m-1}^{(h-1)}(A) \in \mathcal{P}_{m-1}$, $p_{m-1}^{(j)} \in \mathcal{P}_{m-1}$, $(j = 1, 2, \dots, h - 1)$, which interpolates $f - p_{m-1}^{(1)} - \dots - p_{m-1}^{(j-1)}$ in the Hermite sense at the eigenvalues of $H_m^{(j)}$ ($j = 1, 2, \dots, h - 1$), i.e., at the Ritz values of A with respect to $K_m(A, V_m^{(j)}(\cdot, 1))$.

After h restart cycles, the Krylov subspace approximation is given by

$$\hat{f}^{(h)} = V_m^{(h)}(f(H_m^{(h)}) - p_{m-1}(H_m^{(h)}))e_m^{(1)}.$$

The error expression is given in the following.

$$\begin{aligned} E_h &= (f(A) - p_{m-1}(A))v - V_m^{(h)}(f(H_m^{(h)}) - p_{m-1}(H_m^{(h)}))e_m^{(1)} \\ &= \frac{1}{2\pi i} \int_{\Gamma} (f(\lambda) - p_{m-1}(\lambda))[(\lambda I - A)^{-1}v - V_m^{(h)}(\lambda I - H_m^{(h)})^{-1}e_m^{(1)}]d\lambda. \end{aligned}$$

Let

$$\begin{aligned} r_m(\lambda) &= (\lambda I - A)^{-1}v - V_m^{(h)}(\lambda I - H_m^{(h)})^{-1}e_m^{(1)} \\ &= [(\lambda I - A)^{-1} - V_m^{(h)}(\lambda I - H_m^{(h)})^{-1}(V_m^{(h)})^H]v \end{aligned}$$

and

$$G = (\lambda I - A)^{-1} - V_m^{(h)}(\lambda I - H_m^{(h)})^{-1}(V_m^{(h)})^H$$

then $G(\lambda I - A)V_m^{(h)} = 0$. Hence we have for arbitrary $z_m \in \mathbb{C}^m$

$$(\lambda I - A)^{-1}v - V_m^{(h)}(\lambda I - H_m^{(h)})^{-1}e_m^{(1)} = G(v - (\lambda I - A)V_m^{(h)}z_m).$$

Let

$$\begin{aligned} r(\lambda) &= v - (\lambda I - A)V_m^{(h)}z_m = v - (\lambda I - A)[V_k^{(h)}, V_{m-k}^{(h)}] \begin{bmatrix} 0 \\ z_{m-k} \end{bmatrix} \\ &= v - (\lambda I - A)V_{m-k}^{(h)}z_{m-k}. \end{aligned}$$

Since

$$[V_k, V_{m-k}] = \text{Span}\{v, Av, \dots, A^{m-k-1}v, y_1, y_2, \dots, y_k\}$$

then

$$r(\lambda) = v - (\lambda I - A)V_{m-k}^{(h)}z_{m-k} = v - (\lambda I - A)p_{m-k-1}(A)v = p_{m-k}(A)v,$$

where p_{m-k} is the polynomial of degree $m - k$.

To bound G , we recall $\|V_m^{(h)}\| = 1$ and use the estimates $\|(\lambda I - A)^{-1}\| \leq \text{dist}(\lambda, F(A))^{-1}$ and $\|(\lambda I - H_m^{(h)})^{-1}\| \leq \text{dist}(\lambda, F(A))^{-1}$, which follow from [38, Theorem 4.1], where $F(A) = \{x^H Ax : x \in \mathbb{C}^N, \|x\| = 1\}$. We can obtain

$$\|r_m(\lambda)\| \leq 2d^{-1}(\Gamma)\|p_{m-k}(A)\|,$$

where $d(\Gamma)$ is the minimal distance between $F(A)$ and a subset Γ of the complex plane. From [39, Theorem 3.3.3], we know that there exists $0 < q < 1$, such that $\|p_{m-k}\| \leq q\|v\|$. Therefore, we can obtain the bound

$$\|f(A)v - \hat{f}^{(h)}\| \leq \frac{d^{-1}(\Gamma)l(\Gamma)}{\pi} \inf \|f - p_{m-1}\|_{\infty, \Omega} q\|v\|,$$

where $l(\Gamma)$ denotes the length of the contour Γ and $\|\cdot\|_{\infty, \Omega}$ denotes the supremum norm on Ω . The assertion now follows from the convergence rate of best uniform approximation of entire functions of order one by polynomials. In particular, it is known (see [40]) that there exist constants $\tilde{C}$ and γ such that

$$\inf \|f - p_{m-1}\|_{\infty, \Omega} \leq \tilde{C} \frac{\gamma^{m-1}}{(m-1)!}.$$

The proof is complete. $\square$

Corollary 1. *The deflated restarting Arnoldi approximation converges superlinearly for entire functions of order one.*

5. Numerical experiments

In this section we demonstrate the behavior of the deflated restarting Arnoldi approximation for the matrix functions using several examples from the literature. All computations were carried out in MATLAB version 7.6.0 (R2008a) on an Intel E7200 at 2.53 GHz with 2.0 GB of RAM.

Example 1 (*Three-Dimensional Heat Equation*). The numerical experiment is based on one from [4]. Consider the initial boundary value problem

$$\partial_t u - \Delta u = 0 \quad \text{in } \Omega = (0, 1)^3, \quad t > 0 \quad (5.1a)$$

$$u(x, t) = 0 \quad \text{on } \Gamma = \partial\Omega, \quad t > 0 \quad (5.1b)$$

$$u(x, 0) = u_0(x) \quad \text{in } \Omega. \quad (5.1c)$$

When the Laplacian is discretized by the usual seven-point stencil on a uniform grid involving n interior grid points in each Cartesian direction, problem (5.1) reduces to the initial value problem

$$u'(t) = Au(t), \quad t > 0$$

$$u(0) = u_0$$

with an $N \times N$ matrix A ($N = n^3$) and an initial vector u_0 consisting of the values $u_0(x)$ at the grid points x , the solution of which is given by

$$u(t) = f_t(A)u_0 = e^{tA}u_0. \quad (5.2)$$

As in [4], we give the initial vector in terms of its expansion in eigenfunctions of the discrete Laplacian as

$$u_0^{i,j,k} = \sum_{i',j',k'} \frac{1}{i' + j' + k'} \sin(ii'\pi h) \sin(jj'\pi h) \sin(kk'\pi h).$$

Here $h = 1/(n+1)$ is the mesh size and the triple indexing is relative to the lexicographic ordering of the mesh points in the unit cube.

We consider the case $n = 17$ and repeat a calculation in [4], where (5.2) is approximated at $t = 0.1$. We apply the deflated restarting Arnoldi method with restart lengths $m = 10, 15$ and 20 , as well as restarted Arnoldi method, standard (unrestarted) Arnoldi method and two-sided Lanczos method. The resulting error curves are shown in Figs. 1–3.

Example 2. The example is taken from [10]. We consider the type of matrices which are often adopted in the numerical test. The matrix A is obtained by discretizing on the unit square $(0, 1) \times (0, 1)$, with Dirichlet boundary conditions, the second-order differential operator

$$-\Delta + c_1 \frac{\partial}{\partial x} + c_2 \frac{\partial}{\partial y}, \quad c_1, c_2 \in \mathbb{R},$$

where Δ denotes the Laplacian. We introduce a uniform mesh grid with mesh size $h = 1/(n+1)$ and we employ the central differences for discretizing the Laplacian. Since we will consider only cases where the grid-Péclet numbers are greater than 1, we use the upwind differences for the advection terms. So doing we get the $N \times N$ ($N = n^2$) matrix

$$A = \frac{1}{h^2} [(I_n \otimes B) + (C \otimes I_n)] \in \mathbb{R}^{n^2 \times n^2},$$

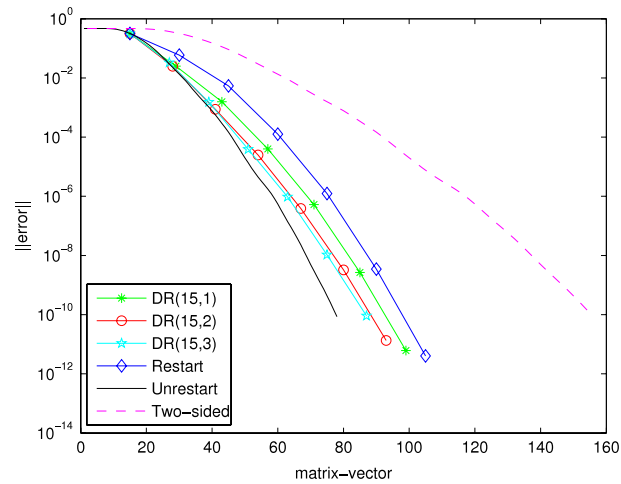


Fig. 1. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 15$ and $k = 1, 2, 3$.

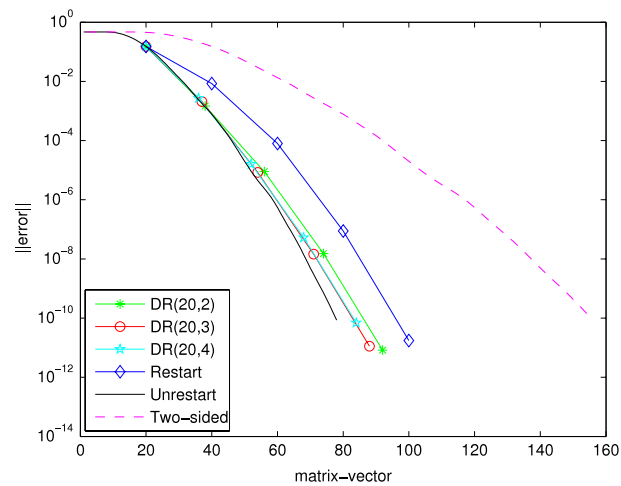


Fig. 2. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 20$ and $k = 2, 3, 4$.

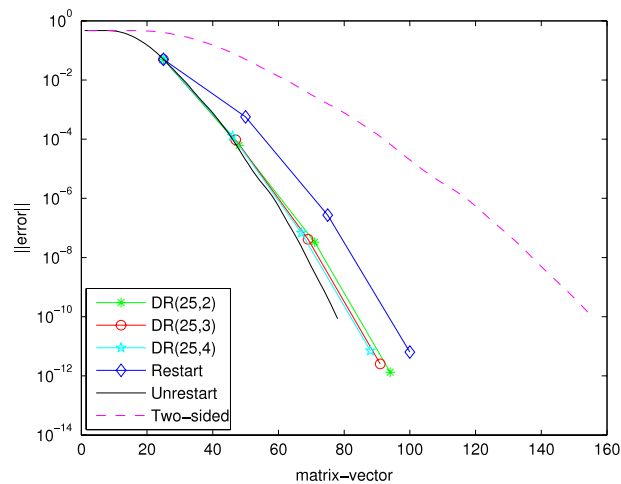


Fig. 3. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 25$ and $k = 2, 3, 4$.

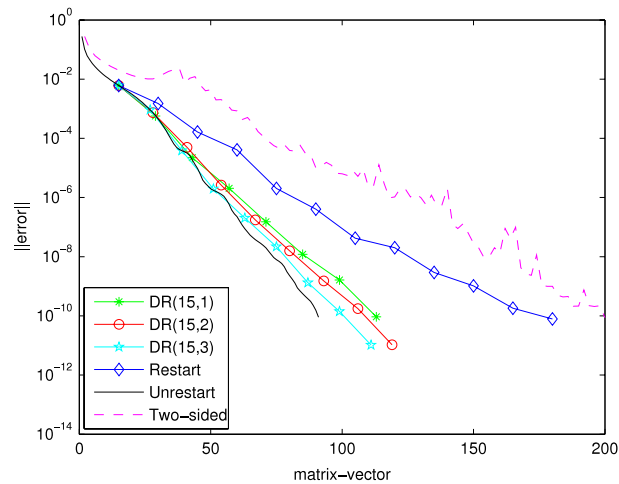


Fig. 4. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 15$ and $k = 1, 2, 3$.

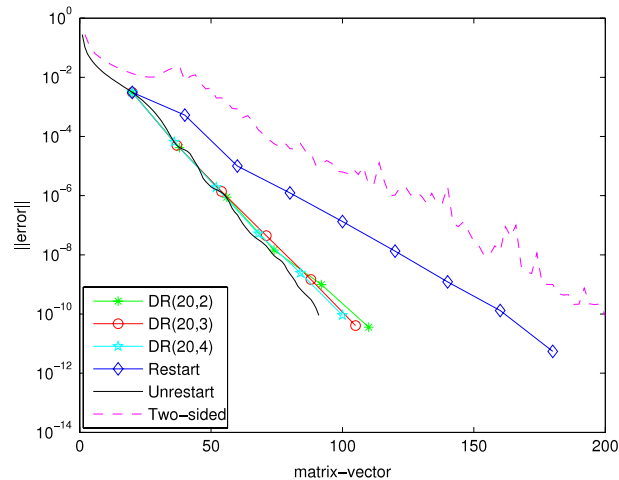


Fig. 5. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 20$ and $k = 2, 3, 4$.

where I_n is the identity matrix of order n ; B and C are tridiagonal matrices defined as

$$B = \begin{bmatrix} 4 + c_1 h + c_2 h & -1 & & \\ -(1 + c_1 h) & 4 + c_1 h + c_2 h & -1 & \\ & -(1 + c_1 h) & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

$$C = \begin{bmatrix} 0 & -1 & & \\ -(1 + c_2 h) & 0 & -1 & \\ & -(1 + c_2 h) & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}.$$

In the experiments we have set $v = [1, 1, \dots, 1]^T / N^{1/2}$.

(1) We firstly consider the function $f(z) = z^{1/2}$. We recall that the function square root denotes the single-valued branch of the many-valued function $z^{1/2}$ that is defined in a domain not containing the origin. We take the square root on the branch such that $1^{1/2} = 1$. The problem examined in this example is the computation of $f(sA)v$, with $s > 0$. As is well known $A^{1/2}$ is well defined. Fixing $n = 30$, $s = 0.001$, $c_1 = 1$, $c_2 = 10$, the error curves of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 15, 20$ and 25 , respectively, are shown in Figs. 4–6.

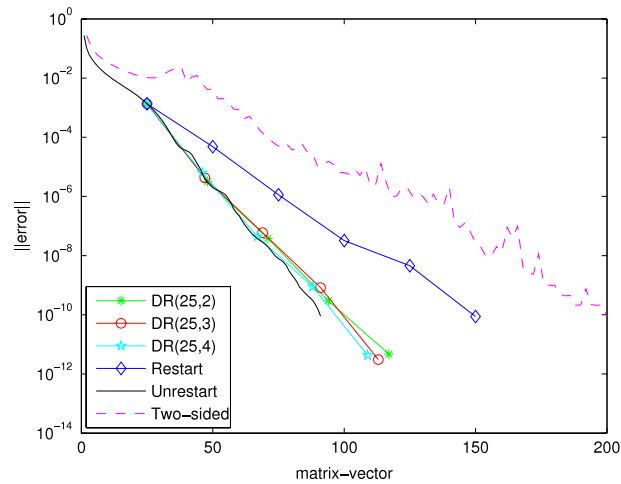


Fig. 6. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 25$ and $k = 2, 3, 4$.

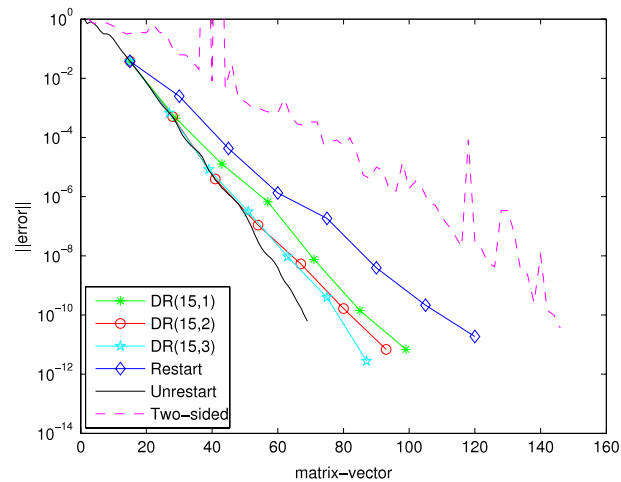


Fig. 7. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 15$ and $k = 1, 2, 3$.

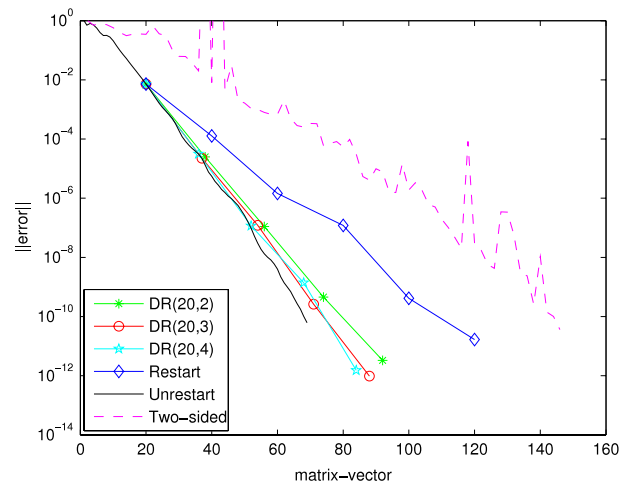


Fig. 8. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 20$ and $k = 2, 3, 4$.

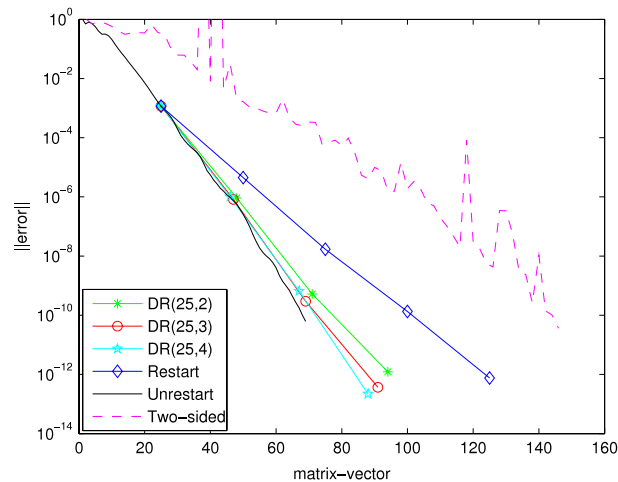


Fig. 9. Error norm histories of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 25$ and $k = 2, 3, 4$.

(2) The function considered is $f(z) = \sin(tz^{1/2})$. In Figs. 7–9 are shown the error curves of the standard (unrestarted) Arnoldi method, two-sided Lanczos method, restarted Arnoldi method and deflated restarting Krylov subspace method with restart length $m = 15, 20$ and 25 , respectively. In the tests we have chosen $n = 20$, $t = 0.1$, $c_1 = 6$, $c_2 = 5$ for the computation of $f(A)v$.

In Examples 1 and 2, we observe that the fastest method is clearly the standard (unrestarted) Arnoldi method, but note that it requires mass storage to store all the basis vectors. In contrast to the restarted Arnoldi method and two-sided Lanczos method, the performance of the deflated restarting Krylov subspace method in this paper is better. This means that our method can be of practical interest. In the experiments, we also find that in most cases the larger k is, the faster convergence is. However, in general, when k is larger, the final precision is lower. Therefore, the choice of k is essential in the deflated restarting Krylov subspace method. However, we have no theoretical result about how to choose k , and this will be the subject of future research.

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