Novel interpretation of contour integral spectral projection methods for solving generalized eigenvalue problems

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Abstract: For generalized eigenvalue problems, we consider computing all eigenvalues located in a certain region and their corresponding eigenvectors. Recently, contour integral spectral projection methods have been proposed for such problems. In this study, from an analysis of the relationship between the contour integral spectral projection and the Krylov subspace, we provide a novel interpretation of these methods. We also propose a new algorithm based on this interpretation.

1 Introduction

We consider computing all eigenvalues located in a certain region and their corresponding eigenvectors $(\lambda_i, \boldsymbol{x}_i), i = 1, 2, \ldots, m$ for the generalized eigenvalue problem in the form

$$A\boldsymbol{x}_i = \lambda_i B\boldsymbol{x}_i, \quad \boldsymbol{x}_i \in \mathbb{C}^n \setminus \{\boldsymbol{0}\}, \quad \lambda_i \in \Omega \subset \mathbb{C}, \tag{1}$$

where $A, B \in \mathbb{C}^{n \times n}$ and the matrix pencil (A, B) is assumed to be regular, i.e., $A - zB$ is nonsingular for some $z \in \mathbb{C}$. Such eigenvalue problems arise in many areas of computational science and engineering.

A powerful algorithm for solving the generalized eigenvalue problem (1) is the contour integral spectral projection method proposed by Sakurai and Sugiura in 2003 [5]. Since then, several authors have actively studied and proposed improved techniques based on the concepts of Sakurai and Sugiura [1, 2, 4, 6].

In this study, we analyze the relationship between the contour integral spectral projection and the Krylov subspace, and provide a novel interpretation of contour integral spectral projection methods. We also propose a new algorithm based on this interpretation.

The remainder of this paper is organized as follows. In Section 2, we briefly describe the basic concepts of contour integral spectral projection methods. In Section 3, we provide a novel interpretation and propose a new algorithm based on this interpretation. In Section 4, we show results from numerical experiments using our proposed algorithm, and finally we draw some conclusions in Section 5.

Throughout this paper, the following notations are used. Let $A = [\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_m] \in \mathbb{C}^{n \times m}$, then $\mathrm{span}\{A\} := \mathrm{span}\{\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_m\}$. Also, let $\mathcal{V}, \mathcal{W}$ be subspaces, then $\mathcal{V} + \mathcal{W}$ denotes the sum of the subspaces of $\mathcal{V}, \mathcal{W}$, i.e., $\mathcal{V} + \mathcal{W} := \{\boldsymbol{v} + \boldsymbol{w} | \boldsymbol{v} \in \mathcal{V}, \boldsymbol{w} \in \mathcal{W}\}$.

Algorithm 1 The Rayleigh-Ritz procedure

Input: m dimensional subspace $\mathcal{S}_m$

Output: Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, m$

  1: Compute the orthonormal basis $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m]$ of the subspace $\mathcal{S}_m$

  2: Compute eigenpairs $(\lambda_i, \boldsymbol{u}_i)$ of the matrix pencil $(W^{\mathrm{H}}AW, W^{\mathrm{H}}BW)$,

     and $\boldsymbol{x}_i = W\boldsymbol{u}_i$ for $i = 1, 2, \ldots, m$

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2   Contour integral spectral projection methods

For solving the generalized eigenvalue problem (1), a contour integral spectral projection method was first introduced by Sakurai and Sugiura in 2003 [5]. For solving (1), they introduced the rational function

$$f(z) := \boldsymbol{u}^{\mathrm{H}}(zB - A)^{-1}\boldsymbol{v}, \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{C}^n \setminus \{\boldsymbol{0}\}, \tag{2}$$

whose poles are eigenvalues λ of the generalized eigenvalue problem; they then considered computing all poles located in Ω.

All poles located in a certain region of an analytic function can be computed by the algorithm in [3], which is based on the Cauchy's integral formula. Applying the algorithm in [3] to the rational function (2), the eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ of the generalized eigenvalue problem (1) can be obtained from the generalized eigenvalue problem with small Hankel matrices

$$H_M := \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{M-1} \\ \mu_1 & \mu_2 & \cdots & \mu_M \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{M-1} & \mu_M & \cdots & \mu_{2M-2} \end{pmatrix}, \quad H_M^{<} := \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_M \\ \mu_2 & \mu_3 & \cdots & \mu_{M+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_M & \mu_{M+1} & \cdots & \mu_{2M-1} \end{pmatrix},$$

whose entries consist of the moments

$$\mu_k := \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma} (z - \gamma)^k f(z)\mathrm{d}z, \quad k = 0, 1, \ldots,$$

where Γ is the positively oriented Jordan curve (the boundary of Ω), and γ is located in Ω. For details, we refer to [5].

Since then, an improvement on the Sakurai and Sugiura's algorithm has been proposed for obtaining more accurate eigenpairs; this is called the CIRR method [6] and is based on using the Rayleigh-Ritz procedure (Algorithm 1). Block variants of the algorithms in [5] and in [6] have also been proposed [1, 2] for the higher stability of the algorithms, especially when many eigenvalues exist in Ω.

Let $V \in \mathbb{C}^{n \times L} \setminus \{O\}$, e.g., a random matrix. Also, let $S = [S_0, S_1, \ldots, S_{M-1}] \in \mathbb{C}^{n \times ML}$, where

$$S_k = [\boldsymbol{s}_k^{(1)}, \ldots, \boldsymbol{s}_k^{(L)}] := \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma} (z - \gamma)^k (zB - A)^{-1} BV\mathrm{d}z, \quad k = 0, 1, \ldots, M - 1. \tag{3}$$

Then, the block CIRR method [1] constructs the ML-dimensional subspace

$$\mathcal{S}_M := \mathrm{span}\{S\} = \mathrm{span}\{\boldsymbol{s}_0^{(1)}, \ldots, \boldsymbol{s}_0^{(L)}, \boldsymbol{s}_1^{(1)}, \ldots, \boldsymbol{s}_1^{(L)}, \ldots, \boldsymbol{s}_{M-1}^{(1)}, \ldots, \boldsymbol{s}_{M-1}^{(L)}\}, \tag{4}$$

Algorithm 2 The block CIRR method

Input: $N, M, L \in \mathbb{N}, V \in \mathbb{C}^{n \times L}, \gamma, (z_j, \omega_j)$ for $j = 1, 2, \ldots, N$
Output: Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, ML$
  1: Solve $Y_j = (z_j B - A)^{-1} V$ for $j = 1, 2, \ldots, N$
  2: Compute $S_k = (1/N) \sum_{j=1}^{N} \omega_j (z_j - \gamma)^k Y_j$ for $k = 0, 1, \ldots, M - 1$
  3: Compute the QR decomposition of $S = [S_0, S_1, \ldots, S_{M-1}] : S = WR$
  4: Compute eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of the matrix pencil $(W^{\mathrm{H}} A W, W^{\mathrm{H}} B W)$,
     and $(\lambda_i, \boldsymbol{x}_i) = (\theta_i, W \boldsymbol{u}_i)$ for $i = 1, 2, \ldots, ML$
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from the Rayleigh-Ritz procedure. The subspace $\mathcal{S}_M$ contains all eigenvectors of (1): $\mathcal{S}_M = \mathrm{span}\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$ for $m \leq ML$. The block CIRR method with $L = 1$ reduces to the CIRR method.

In practice, the computation of the contour integral in (3) is approximated by some numerical integration rule such as the N-point trapezoidal rule

$$S_k \approx \widetilde{S}_k := \frac{1}{N} \sum_{j=1}^{N} \omega_j (z_j - \gamma)^k (z_j B - A)^{-1} BV,$$

where z_j are the quadrature points and ω_j are the corresponding weights. The simple formulation of the block CIRR method is shown in Algorithm 2; for details, we refer to [2, 6].

3 A novel interpretation and a new algorithm

For a generalization of the Jordan canonical form to the matrix pencil, we have the following theorem.

Theorem 1 (Weierstrass canonical form)**.** *Let $zB - A$ be regular. Then, there exist nonsingular matrices $\widetilde{P}, Q \in \mathbb{C}^{n \times n}$ such that*

$$\widetilde{P}(zB - A)Q = \mathrm{diag}(zI_{n_1} - J_1, \ldots, zI_{n_d} - J_d, zN_{d+1} - I_{n_{d+1}}, \ldots, zN_r - I_{n_r}), \quad (5)$$

where J_i, N_i are Jordan blocks, N_i is nilpotent, and I_{n_i} denotes the identity matrix of order n_i.

Based on Theorem 1, in Section 3.1, we provide a novel interpretation of the contour integral spectral projection. In Section 3.2, we propose a new algorithm based on the block Arnoldi method.

3.1 A novel interpretation of the contour integral spectral projection

Since the matrices $\widetilde{P}, Q$ are nonsingular, we define $P = \widetilde{P}^{-1}, \widetilde{Q} = Q^{-1}$. According to the Jordan block structure of (5), we partition row vectors in $\widetilde{P}, \widetilde{Q}$ into $\widetilde{P}_i, \widetilde{Q}_i \in \mathbb{C}^{n_i \times n}$ and column vectors in P, Q into $P_i, Q_i \in \mathbb{C}^{n_i \times n}$, respectively, for $i = 1, 2, \ldots, r$. Then, we can derive the following lemma and theorem.

Lemma 2. Let $\psi_k(z)$ be a k-degree polynomial. Then, we have

$$\frac{1}{2\pi\mathrm{i}} \oint_\Gamma \psi_k(z-\gamma)(zB-A)^{-1}\mathrm{d}z = \psi_k(S_\Gamma)P_\Gamma,$$

where

$$S_\Gamma := \sum_{i:\lambda_i\in\Omega} Q_i(J_i-\gamma I)\widetilde{Q}_i, \quad P_\Gamma := \sum_{i:\lambda_i\in\Omega} Q_i\widetilde{P}_i.$$

Proof. From [2, Theorem 4], we have the following relation

$$\frac{1}{2\pi\mathrm{i}} \oint_\Gamma (z-\gamma)^k(zB-A)^{-1}\mathrm{d}z = \sum_{i:\lambda_i\in\Omega} Q_i(J_i-\gamma I)^k\widetilde{P}_i, \quad k = 0,1,\ldots.$$

Here, since $\widetilde{Q}_iQ_i = I$ and $\widetilde{Q}_iQ_j = O$ for $i \neq j$,

$$\sum_{i:\lambda_i\in\Omega} Q_i(J_i-\gamma I)^k\widetilde{P}_i = \left(\sum_{i:\lambda_i\in\Omega} Q_i(J_i-\gamma I)\widetilde{Q}_i\right)^k \left(\sum_{i:\lambda_i\in\Omega} Q_i\widetilde{P}_i\right) = S_\Gamma^k P_\Gamma.$$

Therefore, Lemma 2 is proved. $\square$

Definition. Let $A \in \mathbb{C}^{n\times n}, B = [\boldsymbol{b}_1, \boldsymbol{b}_2, \ldots, \boldsymbol{b}_l] \in \mathbb{C}^{n\times l}$. Also, let $\mathcal{K}_m(A, \boldsymbol{b}_1)$ be the Krylov subspace defined by

$$\mathcal{K}_m(A, \boldsymbol{b}_1) := \mathrm{span}\{\boldsymbol{b}_1, A\boldsymbol{b}_1, \ldots, A^{m-1}\boldsymbol{b}_1\}$$

Then, the subspace $\mathcal{K}_m^\square(A, B)$ is defined by the sum of the Krylov subspaces, i.e.,

$$\mathcal{K}_m^\square(A, B) := \mathcal{K}_m(A, \boldsymbol{b}_1) + \mathcal{K}_m(A, \boldsymbol{b}_2) + \cdots + \mathcal{K}_m(A, \boldsymbol{b}_l) = \mathrm{span}\{[B, AB, \ldots, A^{m-1}B]\}.$$

Theorem 3. *Let $\mathcal{S}_M$ be the subspace of the block CIRR method defined by (4). Then, we have*

$$\mathcal{S}_M = \mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV).$$

Proof. From the definition of S_k (3) and Lemma 2, we have $S_k = S_\Gamma^k P_\Gamma V$. Therefore,

$$\mathcal{S}_M = \mathrm{span}\{[S_0, S_1, \ldots, S_k]\} = \mathrm{span}\{[P_\Gamma BV, S_\Gamma P_\Gamma BV, \ldots, S_\Gamma^{M-1} P_\Gamma BV]\} = \mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV).$$

Therefore, Theorem 4 is proved. $\square$

Remark. According to Theorem 4, the block CIRR method can be regarded as the Rayleigh-Ritz procedure based on the block Krylov subspace $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$. Here, we note that in the block CIRR method, the basis vectors of $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$ are explicitly computed by (3) and the QR decomposition of S (Algorithm 2).

3.2 Proposal of a new algorithm based on the block Arnoldi method

In Section 3.1, we analyzed the relationship between the contour integral spectral projection and the block Krylov subspace. In this section, we consider applying the block Arnoldi procedure to the block Krylov subspace $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$, and we propose a new algorithm based on the block Arnoldi method.

For the eigenpairs of the generalized eigenvalue problem (1) and matrix multiplications for S_Γ, we have the following two theorems.

Theorem 4. *Let $H_M \in \mathbb{C}^{ML \times ML}$ be the banded Hessenberg matrix obtained from the matrix formula of the block Arnoldi procedure for the block Krylov subspace $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$:*

$$W^{\mathrm{H}} S_\Gamma W = H_M,$$

where columns of W are the orthonormal basis of $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$. Also, let $(\theta_i, \boldsymbol{u}_i)$ be the standard eigenpairs of H_M. Then, in the case of $m \leq ML$, the eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ of the generalized eigenvalue problem (1) are obtained by $(\lambda_i, \boldsymbol{x}_i) = (\theta_i + \gamma, W\boldsymbol{u}_i)$.

Proof. From the definitions of S_Γ and W, Theorem 5 is proved. $\qquad\square$

Theorem 5. *Let $U = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_L], \boldsymbol{u}_i \in \mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$. Then, there exist $(M-1)$-degree polynomials $\psi_{M-1}(z)$ and $\Psi \in \mathbb{C}^{L \times L}$ such that*

$$U = \psi_{M-1}(S_\Gamma) P_\Gamma V \Psi = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \psi_{M-1}(z - \gamma)(zB - A)^{-1} BV \Psi \mathrm{d}z.$$

We can also compute the matrix multiplications $S_\Gamma U$ based on the contour integral as follows:

$$S_\Gamma U = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (z - \gamma)\psi_{M-1}(z - \gamma)(zB - A)^{-1} BV \Psi \mathrm{d}z. \tag{6}$$

Proof. From Lemma 2 and the definition of $\mathcal{K}_M^\square(S_\Gamma, P_\Gamma BV)$, Theorem 6 is proved. $\qquad\square$

Remark. According to Theorems 5 and 6, the generalized eigenvalue problem (1) can be solved by the block Arnoldi method for computing eigenpairs of S_Γ. Here, matrix multiplications for S_Γ can be efficiently computed based on the contour integral (6).

Consequently, we propose a new algorithm based on the block Arnoldi method, as shown in Algorithm 3. Here, the computation of the contour integral is approximated by the N-point trapezoidal rule, just as in the block CIRR method (Algorithm 2).

When the contour integrals are computed without approximation (without numerical integration), the proposed method is mathematically equivalent to the block CIRR method and to the block variant of Hankel-based method proposed in [2]. The algorithm in [4] can also be regarded as a special case of the restarted version of the proposed algorithm with $M = 1$.

We show the contributions to the computational costs of the block CIRR method (Algorithm 2) and the proposed method (Algorithm 3) in Table 1. Here, we assume that $n \gg L, M, N$ and that the QR decomposition of an $n \times m$ matrix requires $2nm^2$ flops.

Algorithm 3 Proposed algorithm based on the block Arnoldi method

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Input: $N, M, L \in \mathbb{N}, V \in \mathbb{C}^{n \times L}, \gamma, (z_j, \omega_j)$ for $j = 1, 2, \ldots, N$
**Output:** Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, ML$
 1: Solve $Y_j = (z_j B - A)^{-1} BV$ for $i = 1, 2, \ldots, N$
 2: $W_0 = (1/N) \sum_{j=1}^{N} \omega_j Y_j$
 3: Compute the QR decomposition of W_0: $W_0 = W_1 R$
 4: Set $\Psi_{1,j} = R^{-1}$ for $j = 1, 2, \ldots, N$
 5: **for** $k = 1, 2, \ldots, M$ **do:**
 6: $\quad \widetilde{\Psi}_{k,j} = (z_j - \gamma) \Psi_{k,j}$ for $j = 1, 2, \ldots, N$
 7: $\quad \widetilde{W}_k = (1/N) \sum_{j=1}^{N} \omega_j Y_j \widetilde{\Psi}_{k,j}$
 8: $\quad$ **for** $i = 1, 2, \ldots, k$ **do:**
 9: $\quad\quad H_{i,k} = W_i^{\mathrm{H}} \widetilde{W}_k$
 10: $\quad\quad \widetilde{\Psi}_{k,j} = \widetilde{\Psi}_{k,j} - \Psi_{i,j} H_{i,k}$ for $j = 1, 2, \ldots, N$
 11: $\quad\quad \widetilde{W}_k = \widetilde{W}_k - W_i H_{i,k}$
 12: $\quad$ **end for**
 13: $\quad$ Compute the QR decomposition of $\widetilde{W}_k$: $\widetilde{W}_k = W_{k+1} H_{k+1,k}$
 14: $\quad \Psi_{k+1,j} = \widetilde{\Psi}_{k,j} H_{k+1,k}^{-1}$ for $j = 1, 2, \ldots, N$
 15: **end for**
 16: Set $W = [W_1, W_2, \ldots, W_M]$ and $H_M = \{H_{i,j}\}_{1 \le i,j \le M}$
 17: Compute eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of H_M, and $(\lambda_i, \boldsymbol{x}_i) = (\theta_i + \gamma, W\boldsymbol{u}_i)$ for $i = 1, 2, \ldots, ML$

Table 1: Main contributions to the computational costs of the block CIRR method and the proposed algorithm. Here, GEP and SEP denote the generalized and standard eigenvalue problems, respectively.
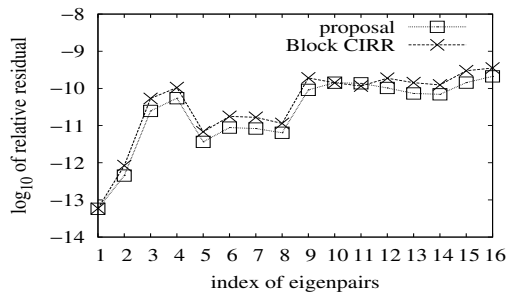
Operation type	Block CIRR		Proposed algorithm	
Solve $(z_j B - A)Y_j = BV$	N	[times]	N	[times]
Mat-Vec for A and B	ML (for A) + ML (for B)	[time]	0	[times]
Solve small eigenvalue problem	GEP: 1	[time]	SEP: 1	[time]
Construct the orthonormal basis	$2nLMN + 2n(LM)^2$	[flops]	$2nL^2MN + 2n(LM)^2$	[flops]
Set small eigenvalue problem	$4n(LM)^2$	[flops]	0	[flops]
Compute eigenvectors	$2nML \times m$	[flops]	$2nML \times m$	[flops]

Table 1 shows that the proposed algorithm is more efficient than the block CIRR method. Note that the proposed algorithm has approximately the same storage requirements as the block CIRR method.

As another advantage of the proposed algorithm, which is based on the block Arnoldi method, it is expected that some improvement techniques used for the (block) Arnoldi method can be applied to the proposed algorithm (Algorithm 3), such as some type of restart techniques, the (block) Lanczos method.
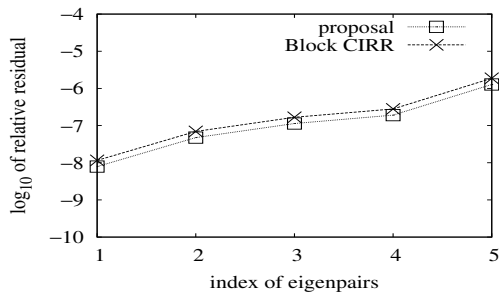
|(a) The first example: MHD|(b) The second example: ESC|

Figure 1: Relative residuals of eigenpairs: $\|A\boldsymbol{x}_i - \lambda_i B\boldsymbol{x}_i\|_2/(\|A\boldsymbol{x}_i\|_2 + |\lambda_i|\|B\boldsymbol{x}_i\|_2)$ from computational results for the two test problems.

4   Numerical examples and results

To confirm that the proposed algorithm (Algorithm 3) can solve generalized eigenvalue problems (1) just as well as the block CIRR method, we provide two numerical examples. The algorithms were implemented in MATLAB R2013a, and the computation of the contour integral was approximated by the N-point trapezoidal rule. The input matrix V was set as a random matrix generated by the MATLAB command "rand", and each linear system was solved by the MATLAB command "\".

The first test problem was taken from a model analysis of dissipative magnetohydro-dynamics (MHD). The obtained matrices A and B were real nonsymmetric and $n = 416$. We set Γ to be the circle with center $\gamma = -0.2 + 0.6\mathbf{i}$ and radius $\rho = 0.05$, and consider finding five eigenvalues located within the circle. We also set $L = 1, M = 5$, and $N = 64$.

The second test problem was taken from an electronic structure calculation (ESC) for a system of silicon. The obtained matrices A and B were Hermitian, and B was positive definite, where $n = 1726$. The eigenvalues are located on the real axis. To find sixteen eigenvalues in the interval $[-0.17, 0.17]$, we set Γ to be the circle with center $\gamma = 0$ and radius $\rho = 0.17$. We also set $L = 4, M = 4$, and $N = 64$.

The relative residuals of eigenpairs for the first and second test problems are shown in Figures 1(a) and 1(b), respectively. Figure 1 shows that the proposed method (Algorithm 3) can compute eigenpairs with approximately the same accuracy as the block CIRR method (Algorithm 2).

5   Conclusions

In this paper, we have provided a novel interpretation of contour integral spectral projection methods for solving the generalized eigenvalue problem (1). We have also proposed a new algorithm based on the block Arnoldi method.

In future, we will propose and analyze efficient improvements in the proposed algorithm based on some techniques that are applied to the block Arnoldi method.

Acknowledgements

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