Contour integrals and Rayleigh-Ritz procedure in nonlinear eigenvalue problems

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Abstract

In this context, we review three algorithms, *i.e.* FEAST algorithm [2, 5, 7], Beyn's algorithm [1] and SS-RR algorithm [9]. We discuss about how they employ contour integrals and what procedure they use to extract eigenvalue/eigenvector approximations.

Contents

1 Introduction

1.1 Contour integrals

In this context, we consider the following *nonlinear eigenvalue* problem. Given a domain $\Omega \subset \mathbb{C}$ and a holomorphic function $T : \Omega \to \mathbb{C}^{m\times m}$, we seek the eigenvalues $\lambda \in \Omega$ and eigenvectors $\boldsymbol{v} \in \mathbb{C}^m$, $\boldsymbol{v} \neq 0$ such that

$$T(\lambda)\boldsymbol{v} = 0.$$

Our aim to obtain all (approximate) eigenvalues and eigenvectors that lie within a given closed contour $\Gamma \in \Omega$, *i.e.* the eigenvalues are filterd by contour Γ. An ideal filter for the eigenvalue problem which maps all wanted eigenvalues eigenvalues to one and all unwanted ones to zero can be derived from the Cauchy integral formula.

Theorem 1 (Cauchy's integral formula)**.** *Let $\Omega \subset \mathbb{C}$ be open and let $f : \Omega \to \mathbb{C}$ be holomorphic on Ω. Let Γ be a simple closed piecewise smooth and positively oriented curve contained in Ω and the inside of Γ is contained in Ω. Then for any $z_0 \in \Gamma$ we have that*

$$f(z_0) = \frac{1}{2\pi\imath}\int_\Gamma \frac{f(z)}{z - z_0}dz.$$

According to Dunford-Schwartz in [3] and [4], the matrix function via Cauchy's intagral formula defined by for a matrix $C \in \mathbb{C}^{m\times m}$, then

$$f(C) = \frac{1}{2\pi\imath}\int_{\Gamma} \frac{f(z)}{zI - C} dz. \tag{1}$$

Eric Polizzi [7] selected this formula (1) with matrix $C = B^{-1}A$ where A, $B \in \mathbb{C}^{m\times m}$ are Hermitian and B is positive definite. Polizzi's FEAST algorithm, which is applicable to linear eigenvalue problems, does not work for nonlinear case.

Remark. In [2], it reads "unfortunately, FEAST algorithm using only the k = 0 moment ($f(z) = 1$) does not work in the case of the nonlinear $T(\lambda)$. When $T(\lambda)$ is nonlinear, taking an initial set of approximate eigenvectors $X(0)$ and refining it using the quadrature approximation of the k = 0 moment, as is done in the linear FEAST algorithm, does not bring the resulting subspace closer to the desired eigenspace." In fact, the main issue in original FEAST algorithm is not $k = 0$ moment, but the expansion of nonlinear function $T(\lambda)$, *i.e.* how to deal with nonlinear function $T(\lambda)$.

For the nonlinear FEAST Algorithm [2], Brendan Gavin *et al.* propose to study the following modified form of the contour integral

$$\frac{1}{2\pi\imath}\int_{\Gamma} \frac{I - T^{-1}(z)T(\lambda)}{z - \lambda} dz. \tag{2}$$

where λ is the current Ritz estimation of an eigenvalue that is inside the contour Γ. This strategy is applicable for polynomial nonlinear eigenvalue problems. In the case of more general (non-polynomial) nonlinear eigenvalue problems, the reduced nonlinear eigenvalue problem will be itself of an arbitrary form, and therefore will require using a Newton- or a projection-type solution method instead of a simple linearization technique (this sentence comes from conclusion of [2]).

Beyn's algorithm [1] and SS-RR algorithm [9] tackle the nonlinear eigenvalue problems by using contour integrals, as well. The difference from FEAST algorithm is that they use the theorem of Keldysh, which provides an **expansion** of $T(z)^{-1}$ and the **residue theorem** to contour integrals

$$\frac{1}{2\pi\imath}\int_{\Gamma} f(z)T(z)^{-1}\hat{V} dz, \qquad \hat{V} \in \mathbb{C}^{m\times l}, \tag{3}$$

which, in consequence, is constructed by chains of generalized eigenvectors [1] (eigenvectors and theirs associated vectors). This strategy makes it possible to tackle nonlinear eigenvalue problems with contour integrals.

1.2 Rayleigh-Ritz procedure

In the first place, we describe Rayleigh-Ritz procedure for solving linear eigenvalue problems. Consider A be an $m \times m$ complex matrix, the procedure can be described as follows:

Algorithm 1. (Rayleigh-Ritz procedure)

1. Select a proper projection subspace $\mathcal{K}$.
2. Compute approximate eigenpairs $(\lambda, \boldsymbol{v})$ satisfying Galerkin condition:

$$A\boldsymbol{v} - \lambda\boldsymbol{v} \perp \mathcal{K}, \qquad \boldsymbol{v} \in \mathcal{K}.$$

Next, we state the Rayleigh-Ritz procedure for solving non-linear eigenvalue problems [9]. Consider the holomorphic function $T : \Omega \to \mathbb{C}^{m\times m}$ that we mentioned above, the approximate eigenspace $\mathcal{V}$ and the chain of generalized eigenvectors $\boldsymbol{v}$, the procedure can be described as follows

Algorithm 2. (Nonlinear Rayleigh-Ritz iterative procedure)

1. Select a proper projection subspace $\mathcal{K}$ that satisfies $\mathcal{V} \subset \mathcal{K}$.

2. Compute approximate eigenpairs $(\lambda, \boldsymbol{v}_0)$ with generalized eigenvectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{n-1}$ where λ inside contour Γ satisfies the Galerkin condition:

$$(T(\lambda)\boldsymbol{v})^{(j)} \perp \mathcal{K}, \qquad \boldsymbol{v}_j \in \mathcal{K}.$$

3. Select approximate eigenpairs that satisfy proper conditions.

We have following comments:

- In Polizzi's FEAST algorithm, the filtering function can be expressed using the spectral decomposition of the Hermitian problem *i.e.* contour itegrals can generate a subspace which contains the desired eigenspace.
- In SS-RR algorithm, there is a theorem (see [9], Theorem 3) which denotes that the subspace containing the eigenspace designate can be generated with contour integrals. The contour integrals are based on Keldysh theorem.

In conclusion, if we want to apply Rayleigh-Ritz approach, we must select a proper subspace which can be generated with contour integrals. Cauchy's integral formula used by FEAST algorithm is possible and contour integrals using Keldysh theorem is possible, which is mentioned and applied in [9].

2 FEAST algorithm

We start with Polizzi's FEAST algorithm [7], which is designed for linear Hermitian generalized eigenvalue problems. Polizzi's FEAST algorithm projects an l-dimensional $(k \leq l \ll m)$ random subspace $\widehat{V}$ onto the subspace spanned by the disired eigenvectors and applies the Rayleigh-Ritz procedure in this subspace to extract eigenvalue/eigenvector approximations. Given a Hermitian generalized eigenvalue problem

$$AX = BX\Lambda, \qquad A, B \in \mathbb{C}^{m\times m}, X \in \mathbb{C}^{m\times k}, \Lambda \in \mathbb{C}^{k\times k},$$

where A is Hermitian and B is a symmetric positive definite, FEAST algorithm can be summarized as follows,

1. Choose a random subspace $\widehat{V} \in \mathbb{C}^{m\times l}$ $(k \leq l \ll m)$.
2. Compute contour integration
$$\widetilde{Q} \approx \frac{1}{2\pi\imath}\int_{\Gamma}(zB - A)^{-1}B\widehat{V}dz.$$
3. Orthogonalize $\widetilde{Q}$ resulting in a matrix with orthonormal columns.
4. Apply Rayleigh-Ritz procedure to get approximate Ritz pairs $(\widetilde{\Lambda}, \widetilde{X})$.
5. If convergence is not reached, then go to Step 1 with $\widehat{V} = \widetilde{X}$.

For Step 2, The FEAST algorithm propsed in [7] applies a numerical quadrature to approximatly compute l vectors at each iteration. We obtain for the approximate subsapce $\widetilde{Q}$:

$$\widetilde{Q} = \sum_{j=1}^{n_e}\omega_j(z_jB - A)^{-1}B\widehat{V},$$

where $\{(z_j, \omega_j)\}_{1\leq j\leq n_e}$ are the nodes and weights of the quadrature. In practice, $\widetilde{Q}$ can be computed by solving small number of independent shifted linear systems over a complex contour:

$$\widetilde{Q} = \sum_{j=1}^{n_e}\omega_j\widetilde{Q}_j,$$

with $\widetilde{Q}_j$ solution of

$$(z_j B - A)\widetilde{Q}_j = B\widehat{V}.$$

Because of these independent linear systems, they can all be solved in parallel. We have following comments:

1. Polizzi's FEAST algorithm [7] is designed for Hermitian generalized eigenvalue problem and the FEAST eigensolver proposed James Kestyn *et al.* [5] for non-hermitian problems, *i.e.* multiple eigenvalues inside the contour, which can be explained by Keldysh theorem for the case of multiple eigenvalues.

2. Brendan Gavin *et al.* proposed a FEAST eigensolver for nonlinear problems [2], which is based on a **modified** form of the contour integrals. It is quite interesting to study the expansion of this modified form (2) to the expansion of the form (3) with Keldysh theorem.

3 Beyn's algorithm

The core of Beyn's algorithm is the theorem of Keldysh, which is empolyed to show that the original nonlinear eigenvalue problem reduces to a linear eigenvalue problem. More specifically, the theorem of Keldysh gives a representation of the singular part of $T(z)^{-1}$ in terms of generalized eigenvectors of T and T^H. For further details of Keldysh theorem, we refer to [1, 6]. In this section, we present Keldysh theorem and Beyn's algorithm. Next, we use Keldysh theorem to form Polizzi's FEAST algorithm and the FEAST algorithm proposed by James Kestyn *et al.*. In the first place, we give the following defintion:

Definition 1. Let $T \in H(\Omega, \mathbb{C}^{m\times m})$ and $\lambda \in \Omega$.

1. **(Root function of T).** A holomorphic vector-valued function $\boldsymbol{v} \in H(\Omega, \mathbb{C}^m)$ is called a root function of T at λ if

$$T(\lambda)\boldsymbol{v}(\lambda) = 0, \qquad \boldsymbol{v}(\lambda) \neq 0.$$

   Let ν, the order of the zero of $T(z)\boldsymbol{v}(z)$ at $z = \lambda$, be a multiplicity of $\boldsymbol{v}$.

2. **(Chain of generalized eigenvectors).** Because $\boldsymbol{v}$ is holomorphic, it admits being expanded as

$$\boldsymbol{v}(z) = \sum_{j=0}^{\infty}(z-\lambda)^j \boldsymbol{v}_j, \qquad \boldsymbol{v}_0 \neq 0.$$

   Consider this expansion of root function with multiplicity ν, we call a tuple $(\boldsymbol{v}_0, \dots, \boldsymbol{v}_{\mu-1})$ a *chain of generalized eigenvectors*(CGE) of T at λ if

$$\boldsymbol{v}(z) = \sum_{j=0}^{\mu-1}(z-\lambda)^j \boldsymbol{v}_j, \qquad 1 \leq \mu \leq \nu.$$

   is a root function of T at λ with multiplicity ν.

3. **(Canonical system of generalized eigenvectors).** Let L be the dimensionality of the eigenspace $N(T(\lambda))$. We assume that for each $\ell = 1, \dots, L$, there is a CGE of t at λ, *i.e.*

$$\boldsymbol{v}^\ell(z) = \sum_{j=0}^{\mu_\ell - 1}(z-\lambda)^j \boldsymbol{v}_j^\ell, \qquad 1 \leq \mu_\ell \leq \nu_\ell,$$

   where $\ell = 1, \dots, L$ and $\boldsymbol{v}_0^1, \dots, \boldsymbol{v}_0^L$ are linearly independent. Then the system

$$V = \left(\ \boldsymbol{v}_j^\ell,\ 0 \leq j \leq \mu_{\ell-1}, 1 \leq \ell \leq L\ \right)$$

   is called a *canonical system of generalized eigenvectors* (CSGE) of T at λ.

Note that the sum of $\mu_\ell(1 \le \ell \le L)$ is the algebraic multiplicity of λ and the number $L = \dim(N(T(\lambda)))$ is the geometric multiplicity.

With the above definition, we can state the following **general** theorem.

Theorem 2 (Keldysh theorem)**.** *We denote $\sigma(T)$ the set of all eigenvalues and $\rho(T) = \Omega \setminus \sigma(T)$ the resolvent set. Let $T \in H(\Omega, \mathbb{C}^{m\times m})$ be given with $\rho(T) \neq \varnothing$. For $\lambda \in \sigma(T)$, let*

$$V = \left(\ \boldsymbol{v}_j^\ell,\ 0 \le j \le \mu_\ell - 1, 1 \le \ell \le L\ \right)$$

be a CSGE of T at λ. Then there exists a CSGE

$$W = \left(\ \boldsymbol{w}_j^\ell,\ 0 \le j \le \mu_\ell - 1, 1 \le \ell \le L\ \right)$$

of T^H at λ, a neighborhood $\mathcal{U}$ of λ and a function $R \in H(\mathcal{U}, \mathbb{C}^{m\times m})$ such that

$$T(z)^{-1} = \sum_{\ell=1}^{L}\sum_{j=1}^{\mu_\ell}(z-\lambda)^{-j}\sum_{i=0}^{\mu_\ell - j}\boldsymbol{v}_i^\ell(\boldsymbol{w}_{\mu_\ell-j-i}^\ell)^H + R(z), \qquad z \in \mathcal{U}\setminus\{\lambda\}. \tag{4}$$

The system W for which (4) holds is the unique CSGE of T^H at λ that satisfies that the multiplicity of $\boldsymbol{v}$ is equal to the multiplicity of $\boldsymbol{w}$ and the following condition

$$\sum_{\alpha=0}^{j}\sum_{\beta=1}^{m_s}(\boldsymbol{w}_{j-\alpha}^\ell)^H T_{\alpha+\beta}\boldsymbol{v}_{m_s-\beta}^s = \delta_{s\ell}\delta_{0j}, \qquad 0 \le j \le m_\ell - 1,\ 1 \le \ell, s \le L,$$

where

$$T_j = \frac{1}{j!}T^{(j)}(\lambda), \qquad j \ge 0.$$

Keldysh theorem provides an expansion of $T(z)^{-1}$ in a neighborhood $\mathcal{U} \subset \Omega$ of an eigenvalue $\lambda \in \Omega$ in terms of generalized eigenvectors of $T(z)$ and its Hermitian transpose $T^H(z)$. For all eigenvalues λ_n, $n = 1, \ldots, n(\mathcal{C})$ inside a compact set $\mathcal{C} \subset \mathcal{U} \subset \Omega$, We can obtain a similar expansion from Keldysh theorem

$$T(z)^{-1} = \sum_{n=1}^{n(\mathcal{C})}\sum_{\ell=1}^{L_n}\sum_{j=1}^{\mu_{\ell,n}}(z-\lambda_n)^{-j}\sum_{i=0}^{\mu_{\ell,n}-j}\boldsymbol{v}_i^{\ell,n}(\boldsymbol{w}_{\mu_{\ell,n}-j-i}^{\ell,n})^H + R(z), \qquad z \in \mathcal{U}\setminus\{\lambda_1, \ldots, \lambda_n\}. \tag{5}$$

For more details, see Corollary 2.8 in [1].

Next, we give the following proporsition and theorem:

Proposition 1 (The residue of an analytic function at a pole singlarity)**.** If z_0 is a pole singularity of order k of analytic function f then

$$\mathrm{Res}(f, z_0) = \lim_{z\to z_0}\frac{[(z-z_0)^k f(z)]^{(k-1)}}{(k-1)!}.$$

Theorem 3 (The Residue theorem)**.** *Let $U \subset \mathbb{C}$ be a simply connected and open set and let $\{\lambda_1, \ldots, \lambda_n\} \subset U$ be a finite collection of points in U. Let f be a complex function that is holomorphic on $U\setminus\{\lambda_1, \ldots, \lambda_n\}$ and let Γ be a simple closed, piecewise smooth positively oriented curve in U enclosing (but not passing through) the points $\{\lambda_1, \ldots, \lambda_n\}$. Then*

$$\oint_\Gamma f(z)\,dz = 2\pi\imath\sum_{k=1}^{n}\mathrm{Res}(f, \lambda_k).$$

Now consider a simple closed curve $\Gamma \subset \Omega$ and combine (5) and the above residue theorem, an easy consequence is the following result.

Theorem 4. *Let $T \in H(\Omega, \mathbb{C}^{m\times m})$ has no eigenvalues on the contour $\Gamma \subset \Omega$ and denote by λ_n, $n = 1, \dots, n(\Gamma)$ the eigenvalues in the interior int$(\Gamma) \subset \Omega$. Then with the CSGEs from (5) we have for any $f \in H(\Omega, \mathbb{C})$*

$$\frac{1}{2\pi\imath}\int_\Gamma f(z)T(z)^{-1} = \sum_{n=1}^{n(\Gamma)}\sum_{\ell=1}^{L_n}\sum_{j=1}^{\mu_{\ell,n}} \frac{f^{(j-1)}(\lambda_n)}{(j-1)!}\sum_{i=0}^{\mu_{\ell,n}-j} \boldsymbol{v}_i^{\ell,n}(\boldsymbol{w}_{\mu_{\ell,n}-j-i}^{\ell,n})^H. \tag{6}$$

This theorem shows that the original nonlinear eigenvalue problem reduces to a linear eigenvalue problem of dimension $n(\Gamma)$.

Assume that $n(\Gamma)$ is not larger than the system dimension m. In large-scale problems we actually expect to have $n(\Gamma) \ll m$. In this case, Beyn's algorithm uses two contour integrals with $f(z) = 1$ and $f(z) = z$ respectively and the *singular value decomposition* (SVD) to reach convergence. FEAST algorithm for Hermitian generalized eigenvalue problem and for non-Hermitian generalized eigenvalue problem can be derived from (6).

3.1 Towards Polizzi's FEAST algorithm

In Polizzi's FEAST algorithm [7], $T(\lambda) = A - \lambda B$, where A is Hermitian matrix and B is a symmetric positive definite matrix. Then we have

$$T = T^H$$

and

$$\mu_{\ell,n} = 1,$$

where $\ell = 1, \dots, L$, $n = 1, \dots, n(\Gamma)$. Then (6) simplifies to

$$\frac{1}{2\pi\imath}\int_\Gamma f(z)T(z)^{-1} = \sum_{n=1}^{n(\Gamma)}\sum_{\ell=1}^{L_n} \boldsymbol{v}_0^{\ell,n}(\boldsymbol{v}_0^{\ell,n})^H.$$

This Equation shows that the desired eigenspace can be generated with contour integrals and Rayleigh-Ritz procedure can be applied.

3.2 Towards James's FEAST algorithm

In James's FEAST algorithm [5] which is designed for non-Hermitian eigenvalue problems, (6) shows that $T(z)^{-1}$ contains left eigenvector subspace and right eigenvector subspace. For this case, we can apply Rayleigh-Ritz procedure with Petrov-Galerkin condition to solve this eigenvalue problem.

4 SS-RR algorithm

SS-RR algorithm [9] is based on Keldysh theorem, as well. The difference from Beyn's algorithm is that SS-RR algorithm applies nonlinear Rayleigh-Ritz iterative procedure to reach convergence. In fact, this iterative procedure is mentioned in [9] but not proven. In [8], this is a similar iterative procedure is proven for generalized eigenvalue problem

$$A\boldsymbol{x} = \lambda B\boldsymbol{x},$$

where A, $B \in \mathbb{R}^{m\times m}$ are symmetric and B is positive definite. It is worth studying Rayleigh-Ritz type method with contour integrals for nonlinear eigenvalue problems.

5 Conclusion

The theorem of Keldysh shows that the singular part (containing desired eigenvalues) of one general eigenvalue problem

$$T(z)\boldsymbol{v} = 0, \qquad \boldsymbol{v} \in C^m, \ v \neq 0, \ z \in \Omega,$$

where $T : \Omega \to \mathrm{C}^{m\times m}$ is assumed to be holomorphic in some domain $\Omega \subset \mathbb{C}$, can be represented by generalized eigenvectors of T and T^H. For different types of problems, there are different algorithms.

1. For linear Hermitian generalized eigenvalue problems, Rayleigh-Ritz procedure is applied to reach convergence [7].
2. For linear non-Hermitian generalized eigenvalue problems, Rayleigh-Ritz procedure with Petrov-Galerkin condition is applied to reach convergence [5].
3. For general polynomial nonlinear eigenvalue problems, a modified form of the contour integrals is proposed and Rayleigh-Ritz procedure is kept to reach convergence [2].
4. For gneneral nonlinear eigenvalue problems, Beyn's algorithm uses two contour integrals and SVD to reach convergence [1] and SS-RR algorithm uses as many contour integrals as necessary and nonlinear Rayleigh-Ritz iterative procedure to reach convergence [9].

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