A contour-integral based method for counting the eigenvalues inside a region in the complex plane

Guojian Yin

Shenzhen Institutes of Advanced Technology,
Chinese Academy of Sciences

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Consider generalized eigenvalue problem

$$Ax = \lambda Bx$$

Goal: counting the eigenvalues inside a given circle Γ.

When $A = A^*$, $B = B^*$, and $B > 0$ → λ_i are real-valued.

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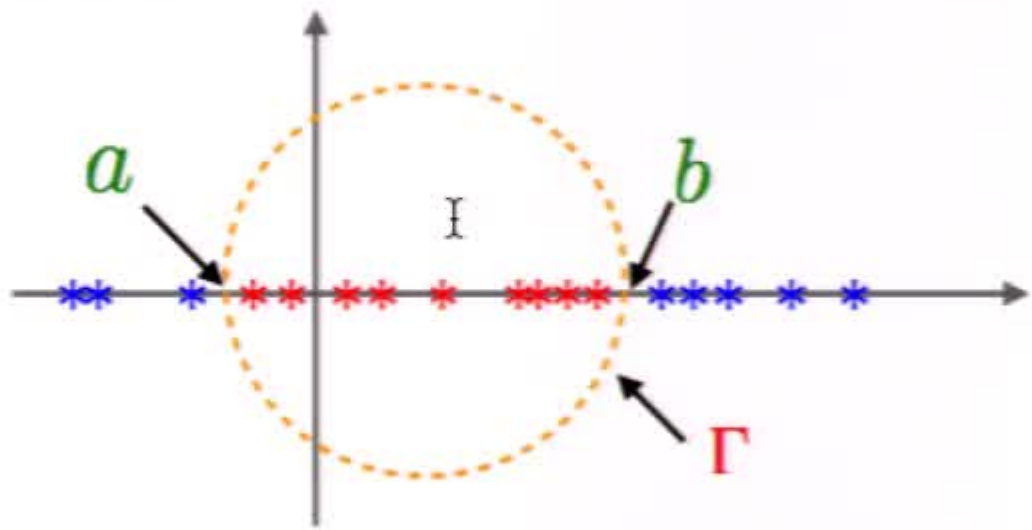
Hermitian problem



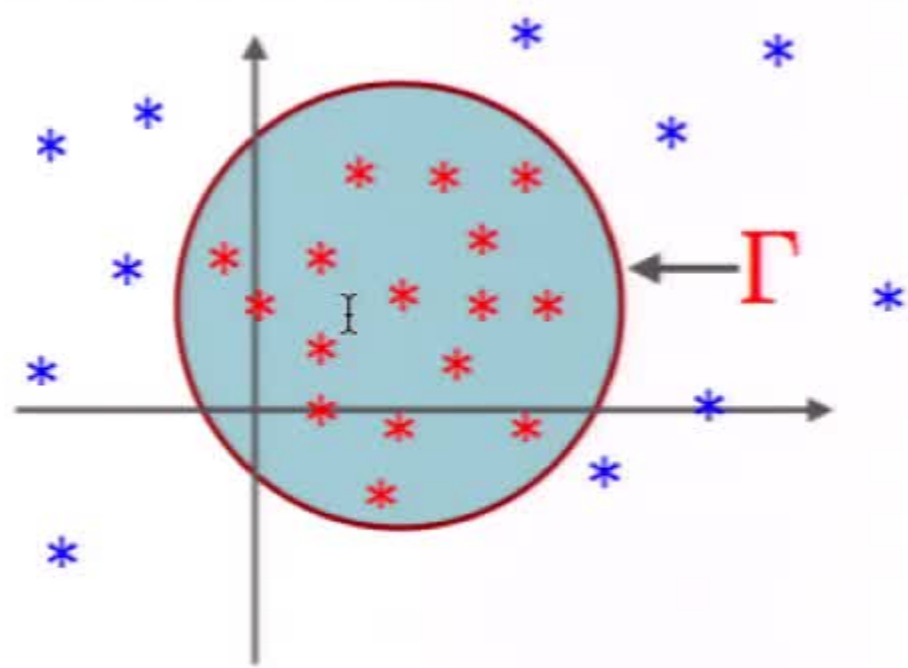
The standard method for Hermitian problem:

Compute $A - aB = L_a D_a L_a^*$ and $A - bB = L_b D_b L_b^*$

Let μ_a and μ_b be the Nos of negative entries of $\mathrm{diag}(D_a)$ and $\mathrm{diag}(D_b)$.

Sylvester law of inertia → #eigs inside $[a, b] = \mu_b - \mu_a$

However, when it comes to non-Hermitian problems ?



Outline

- Estimating the number of eigenvalues inside Γ;
- Finding an upper bound of the number of eigenvalue inside Γ;
- Counting the eigenvalues inside Γ;
- An application.

Estimating the number of eigenvalues inside Γ

Consider the most common generalized eigenvalue problems

matrix pencil $zB - A$ is regular ⟸ $\det(A - zB) \not\equiv 0$

Weierstrass canonical form for the regular matrix pencil:

Theorem: Let $zB - A$ be a regular matrix pencil of order n. Then there exist nonsingular matrices $S, T \in \mathbb{C}^{n\times n}$ such that

$$TAS = \begin{bmatrix} J_d & 0 \\ 0 & I_{n-d} \end{bmatrix} \quad \text{and} \quad TBS = \begin{bmatrix} I_d & 0 \\ 0 & N_{n-d} \end{bmatrix},$$

where J_d is a $d \times d$ matrix in Jordan canonical form, N_{n-d} is an $(n-d)\times(n-d)$ Nilpotent matrix.

Suppose the considered eigenproblem is semi-simple.

↓

J_d is a diagonal matrix and N_{n-d} is a zero matrix.

Let

$$J_d = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d \end{bmatrix},$$

where λ_i are eigenvalues, are not necessarily distinct and can be repeated according to their multiplicities.

Let $Y_p \sim \mathsf{N}_{n\times p}$, an $n \times p$ random matrix with i.i.d. Gaussian entries.

One can easily verify that

$$\begin{aligned}\frac{1}{p}\mathbb{E}[\mathrm{trace}(Y_p^* Q Y_p)] &= \mathrm{trace}(Q) = \mathrm{trace}(S_{(:,1:s)}(S^{-1})_{(1:s,:)}) \\ &= \mathrm{trace}((S^{-1})_{(1:s,:)}S_{(:,1:s)}) \\ &= \mathrm{trace}(I_s) = \boxed{s}\end{aligned}$$

➡ $s_0 := \frac{1}{p}\mathrm{trace}(Y_p^* Q Y_p)$ gives estimation of s.

Experiment 1:

Test matrices: downloaded from the Matrix Market collection.

Table 1: A group of data selected from the Matrix Market.

No.	Matrix	Size	nnz	Porperty	Condition Number
1	A: BFW398A	398	3678	unsymmetric	7.58×10^3
	B: BFW398B	398	2910	symmetric indefinite	3.64×10^1
2	A: BFW782A	782	7514	unsymmetric	4.63×10^3
	B: BFW782B	782	5982	symmetric indefinite	3.05×10^1
3	A: PLAT1919	1919	17159	symmetric indefinite	1.40×10^{16}
	B: PLSK1919	1919	4831	skew symmetric	1.07×10^{18}
4	A: BCSSTK13	2003	42943	symmetric positive definite	4.57×10^{10}
	B: BCSSTM13	2003	11973	symmetric positive semi-definite	Inf
5	A: BCSSTK27	1224	28675	symmetric positive definite	7.71×10^4
	B: BCSSTM27	1224	28675	symmetric indefinite	1.14×10^{10}
6	A: MHD3200A	3200	68026	unsymmetric	2.02×10^{44}
	B: MHD3200B	3200	18316	symmetric indefinite	2.02×10^{13}
7	A: MHD4800A	4800	102252	unsymmetric	2.54×10^{57}
	B: MHD4800B	4800	27520	symmetric indefinite	1.03×10^{14}

They are the real-world GEP coming from scientific and engineering applications.

No.	γ	ρ	s	s_0
1	-5.0×10^5	2.0×10^5	123	122
2	-6.0×10^5	3.0×10^5	230	231
3	0	1.0×10^{-3}	270	277
4	0	6.0×10^5	172	173
5	5.0×10^3	2.0×10^3	107	107
6	-4.0×10^1	3.0×10^1	162	118
7	-6.0	3.0	169	3667

Finding an upper bound of the number of eigenvalues inside Γ

For the contour-integral based eigensolvers, such as SS and FEAST, we must select a parameter s_1 satisfying $s_1 \geq s$ before starting.

An algorithm based on s_0 to seek an s_1 that is slightly $> s$ (Yin, Chan and Yeung '15)

Recall

$$Q = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz = S_{(:,1:s)} (S^{-1})_{(1:s,:)}.$$

Thus,

$Q^2 = Q$ ➡ Q is a spectral projector onto $\text{span}\{S_{(:,1:s)}\}$.

Let $s^\dagger$ be a positive integer and $Y_{s^\dagger} \sim \mathsf{N}_{n\times s^\dagger}(0,1)$. Consider

$$U_{s^\dagger} = QY_{s^\dagger} = S_{(:,1:s)}(S^{-1})_{(1:s,:)}Y_{s^\dagger}.$$

→ $U_{s^\dagger}$ is the projection of $Y_{s^\dagger}$ onto $\mathrm{span}\{S_{(:,1:s)}\}$

$\mathrm{rank}(U_{s^\dagger}) \leq s$

$\mathrm{rank}(U_{s^\dagger}) = s^\dagger$ → $s^\dagger \leq s$

$\mathrm{rank}(U_{s^\dagger}) < s^\dagger$ → $s = \mathrm{rank}(U_{s^\dagger})$

Lemma: Let $Y \in \mathbb{R}^{n\times t}$. If the entries of Y are random numbers from a continuous distribution and that they are independent and identically distributed (i.i.d.), then the matrix $(S^{-1})_{(1:t,:)}Y$ is almost surely nonsingular.

Function $[U_1, s_1] = \text{SEARCH}(A, B, \Gamma, \alpha, p, \delta)$

1. Pick $Y_p \sim \mathsf{N}_{n\times p}(0,1)$ and compute $U = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz Y_p$ by the q-point Gauss-Legendre quadrature rule.
2. Set $s_0 = \lceil \frac{1}{p} \text{trace}(Y_p^* U) \rceil$ and $s^\star = \min(\max(p, s_0), n)$.
3. If $s^\star > p$
4. Pick $\hat{Y} \sim \mathsf{N}_{n\times(s^\star - p)}(0,1)$ and compute $\hat{U} = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz \hat{Y}$ by the q-point Gauss-Legendre quadrature rule.
5. Augment $\hat{U}$ to U to form $U = [U, \hat{U}] \in \mathbb{C}^{n\times s^\star}$.
6. Else
7. Set $s^\star = p$.
8. End
9. Compute the rank-revealing QR decomposition of U with column pivoting strategy: $U\Pi = [U_1, U_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}$, here $\|R_{22}\| \leqslant \delta$.
10. Set $s_1 = \text{rank}(R_{11})$.
11. If $s_1 < s^\star$, stop. Otherwise, set $p = s_1$ and $s^\star = \lceil \alpha s_1 \rceil$. Then go to Step 3.

Experiment 2:

No.	γ	ρ	s	s_0	s_1
1	-5.0×10^5	2.0×10^5	123	122	137
2	-6.0×10^5	3.0×10^5	230	231	262
3	0	1.0×10^{-3}	270	277	328
4	0	6.0×10^5	172	173	183
5	5.0×10^3	2.0×10^3	107	107	118
6	-4.0×10^1	3.0×10^1	162	118	178
7	-6.0	3.0	169	3667	186

Counting the eigenvalues inside Γ

Recall the spectral operator defined by contour integral:

$$Q = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz = S \left[\frac{1}{2\pi\sqrt{-1}} \oint_\Gamma D(z) dz \right] S^{-1} = S \begin{bmatrix} I_s & 0 \\ 0 & 0 \end{bmatrix} S^{-1}$$

residue theorem

Note that

$$D(z) = \begin{bmatrix} (zI_d - J_d)^{-1} & 0 \\ 0 & 0 \end{bmatrix},$$

and

$$(zI_d - J_d)^{-1} = \begin{bmatrix} \frac{1}{z-\lambda_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{z-\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{z-\lambda_d} \end{bmatrix}.$$

$$Q = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz = S \left[\frac{1}{2\pi\sqrt{-1}} \oint_\Gamma D(z) dz \right] S^{-1} = S \begin{bmatrix} I_s & 0 \\ 0 & 0 \end{bmatrix} S^{-1}$$

Applying the Gauss-Legendre quadrature rule to

$$\frac{1}{2\pi\sqrt{-1}} \oint_\Gamma D(z) dz \approx D = \frac{1}{2} \sum_{j=1}^{q} \omega_j (z_j - c) D(z_j).$$

We see that $D_{(i,i)} = \widetilde{\psi}(\lambda_i), \quad i = 1, \ldots, d$

λ_i inside Γ

$\Re[D_{(i,i)}] \geqslant \frac{1}{2}$

λ_i inside Γ

$\Re[D_{(i,i)}] < \frac{1}{2}$

Getting s via counting the $\Re[D_{(i,i)}]$ that are $\geqslant \frac{1}{2}$

Call function $[U_1, s_1] = \textsc{Search}(A, B, \Gamma, \alpha, p)$

Theorem: Let U_1 be the projection matrix computed by function $\textsc{Search}$. Define projection matrix

$$U_2 = QU_1 = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz U_1,$$

and compute it by the q-point Gauss-Legendre quadrature rule to get approximation $\widetilde{U}_2$. Define the $s_1 \times s_1$ matrix

$$M = U_1^* \widetilde{U}_2,$$

then the eigenvalues of M are $\{D_{(i,i)}\}_{i \in \mathcal{I}}$, where $\mathcal{I}$ is an index set and its cardinality is s_1, and $\{1, 2, \ldots, s\} \subset \mathcal{I}$.

↓

Getting s by counting the $\Re[\mathtt{eig}(M)]$ that $\geqslant \frac{1}{2}$.

Experiment 3:

Let $\Lambda = \mathtt{diag}([0.1:0.1:0.8])$, $S = \mathtt{rand}(8)$, $Y = \mathtt{randn}(8,6)$. Define

$$A = S\Lambda S^{-1}, \qquad B = \mathtt{eye}(8).$$

Eigs: 0.1, 0.2, 0.3, 0.4, 0.5, ..., 0.8 $\qquad$ Γ: $c = 0$, $\rho = 0.401$.

i	$\Re[(D_{(i,i)})]$	$\Re[\mathtt{eig}(M)]$
1	1.000000000003949	1.000000000003965
2	1.000000000000000	1.000000000000012
3	0.999999999999999	0.999999999999999
4	0.801581787659601	0.801581787659610
5	0.000000002525684	0.000000002525620
6	0.000000000004379	0.000000000004380
7	0.000000000000001	
8	−0.000000000000051	

A contour-integral based method for computing the number of eigenvalues inside Γ

Function $s = \text{COUNT\_EIGS}(A, B, \Gamma, \alpha, p)$
1. Call $[U_1, s_1] = \text{SEARCH}(A, B, \Gamma, \alpha, p)$;
2. Compute $U_2 = QU_1 = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz U_1$ by the q-point Gauss-Legendre quadrature rule to get $\widetilde{U}_2$, and set $M = U_1^* \widetilde{U}_2$;
3. Compute the eigenvalues of M, and set s to be the number of the computed eigenvalues whose real parts are larger than $\frac{1}{2}$.

Experiment 4: Determine the number of eigenvalues inside Γ

No.	c	ρ	s	s_0	s_1	Cont_Eigs
1	-5.0×10^5	2.0×10^5	123	122	137	123
2	-6.0×10^5	3.0×10^5	230	231	262	230
3	0	1.0×10^{-3}	270	277	328	270
4	0	6.0×10^5	172	173	183	172
5	5.0×10^3	2.0×10^3	107	107	118	107
6	-4.0×10^1	3.0×10^1	162	118	178	162
7	-6.0	3.0	169	3667	186	169

s: the exact number of eigenvalues inside Γ;

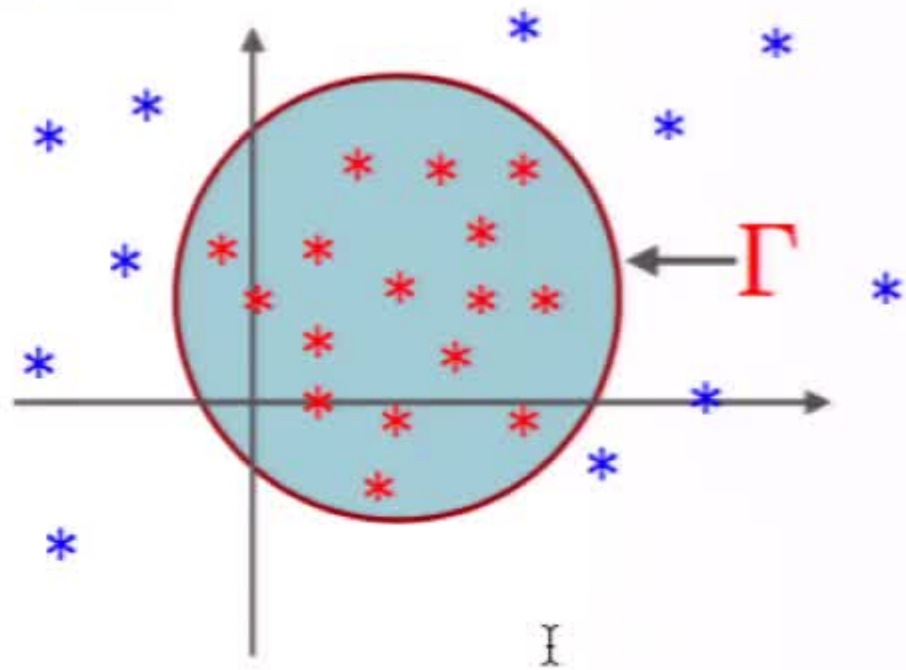
s_0: the estimation of s;

s_1: an upper bound of s;

Cont_Eigs: the number of $\Re[\texttt{eig}(M)] \geqslant \frac{1}{2}$.

An application

The contour-integral based eigensolvers are recent efforts for computing the eigenvalues inside a given curve.



Attractive feature : they are very easily parallelizable.

Drawback: the number s has to be known in advance.

The first reason → Choose a starting matrix $Y \in \mathbb{R}^{n \times s_1}$ satisfying $s_1 \geq s$.

The second reason → Guarantee all desired eigenvalues are found

$$[U_1, s_1] = \textsc{Search}(A, B, \Gamma, \alpha, p)$$

$$s = \textsc{Count\_Eigs}(A, B, \Gamma, \alpha, p)$$

A FEAST algorithm for non-Hermitian problems (Yin, Chan and Yeung '15)

$$U = QY, \quad Y \sim \mathsf{N}_{n\times s_1}(0,1), s_1 \geq s.$$

Let

$$\widetilde{A} = (BU)^* AU \quad \text{and} \quad \widetilde{B} = (BU)^* BU$$

Theorem: Let $\{(\tilde{\lambda}_i, \mathbf{y}_i)\}_{i=1}^{s}$ be eigenpairs of projected eigenproblem $\widetilde{A}\mathbf{y} = \tilde{\lambda}\widetilde{B}\mathbf{y}$, then $\{(\tilde{\lambda}_i, U\mathbf{y}_i)\}_{i=1}^{s}$ are exact eigenpairs of $Ax = \lambda Bx$ that are located inside Γ.

U_2 is also a projection matrix

Function $[\Lambda, X] = \textsc{Ciop}(A, B, \Gamma, \alpha, p, max\_iter)$

1. Call $[U_1, s_1] = \textsc{Search}(A, B, \Gamma, \alpha, p)$.
2. Compute $U_2 = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz U_1$ by the Gauss-Legendre quadrature rule.
3. Set $M = U_1^* U_2$, set s to be the number of eigenvalues of M satisfying $\Re[\mathtt{eig}(M)] \geqslant \frac{1}{2}$.
4. For $k = 2, \ldots, max\_iter$
5. Form $\tilde{A} = (BU_k)^* A U_k$ and $\tilde{B} = (BU_k)^* B U_k$.
6. Solve the projected eigenproblem $\tilde{A}\mathbf{y} = \lambda \tilde{B}\mathbf{y}$ of size s_1 to obtain eigenpairs $\{(\lambda_i, \mathbf{y}_i)\}_{i=1}^{s_1}$. Set $\mathbf{x}_i = U_k \mathbf{y}_i, i = 1, 2, \ldots, s_1$.
7. If there are s eigenpairs $(\lambda_i, \mathbf{x}_i)$ satisfy convergence criteria, stop. Otherwise, compute $U_{k+1} = \frac{1}{2\pi\sqrt{-1}} \oint_\Gamma (zB - A)^{-1} B dz U_k$ by the Gauss-Legendre quadrature rule.
8. End