Resolvent sampling based Rayleigh–Ritz methods using iterative solvers for the numerical solution of Hermitian linear eigenvalue problems

Project TM

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Outline:

Physical motivation

Theoretical background:
Resolvent sampling Rayleigh–Ritz methods

Research questions

1) Analysis according to filter functions
2) Condition number
3) Influence of iterative solver on eigenvalue residual

Physical motivation

Search for eigenpairs of large Hermitian matrices in a specified domain $\Omega \subset \mathbb{C}$:

Spectral analysis of superconducting cuprates

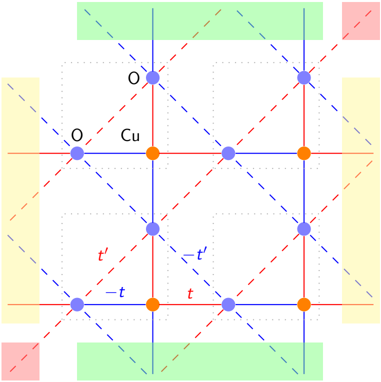


Figure: Illustration of the physical model of a copperoxide flake.

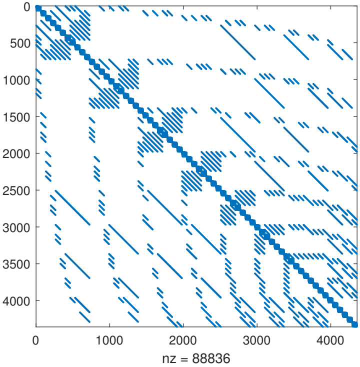


Figure: Sparsity of the examined matrix.

Spectrum of the matrix and investigated spectral domain

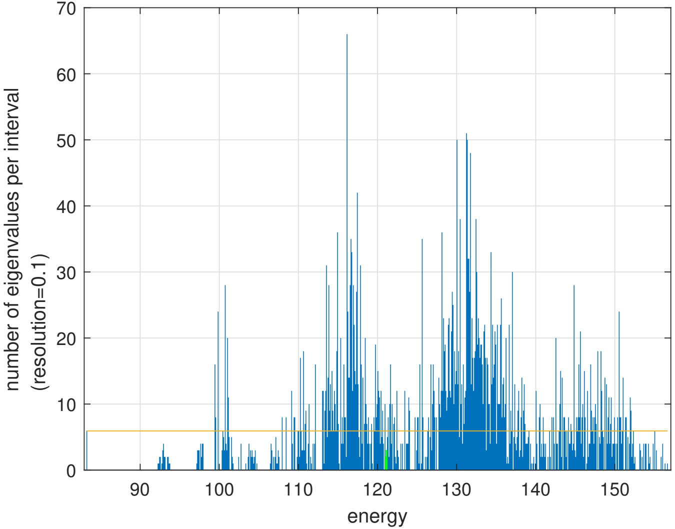


Figure: Spectrum of the analyzed matrix.

Hubbard model (Emery model)

$$\underbrace{H = \varepsilon_{Cu} \sum_{Cu,\sigma} n_{Cu,\sigma} + \varepsilon_O \sum_{O,\sigma} n_{O,\sigma}}_{\text{on–site energy}}$$

$$\underbrace{+t \sum_{\langle OCu\rangle,\sigma} \pi(\langle OCu\rangle) c^\dagger_{O\sigma} c_{Cu\sigma} + h.c. + t' \sum_{\langle OO'\rangle,\sigma} \pi(\langle OO'\rangle) c^\dagger_{O\sigma} c_{O'\sigma}}_{\text{kinetic part}}$$

$$\underbrace{+U_O \sum_{O} n_{O\uparrow} n_{O\downarrow} + U_{Cu} \sum_{Cu} n_{Cu\uparrow} n_{Cu\downarrow} + U_{OCu} \sum_{\langle OCu\rangle,\sigma} n_{O\sigma} n_{Cu\overline{\sigma}}}_{\text{Coulomb interaction}}$$

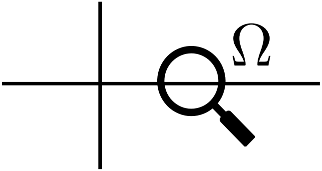
$$\varepsilon_{Cu} = 0, \quad \varepsilon_O = 3.6, \quad t = 1.3, \quad t' = 0.65,$$
$$U_O = 4, \quad U_{Cu} = 10.5, \quad U_{OCu} = 1.2, \quad U_{OO'} = 0.$$

Theoretical background:
Resolvent sampling Rayleigh–Ritz methods

Rayleigh–Ritz projection method

1. Orthonormal basis u_ι that approximates desired eigenspace
2. Form projection operator $U = [u_1, \ldots, u_r]$
3. Perform projection $\mathbb{C}^{r \times r} \ni \tilde{A} := U^* A U$.
4. Solve eigenproblem of $\tilde{A}$ to gain eigenpairs $(\tilde{\lambda}_\iota, \tilde{u}_\iota)$
5. Gain Ritz pairs $(\tilde{\lambda}_\iota, \tilde{v}_\iota)$ with $\tilde{v}_\iota = U\tilde{u}_\iota$ as approximation of desired eigenpairs (λ_ι, v_ι)

Contour integral method



Projector onto desired eigenspace:

$$\frac{1}{2\pi \mathrm{i}} \oint_{\partial\Omega} \frac{1}{z\mathbb{1} - A} dz = \frac{1}{2\pi \mathrm{i}} \sum_{\iota} \oint \frac{1}{z - \lambda_\iota} v_\iota v_\iota^* = \sum_{\lambda_\iota \in \Lambda} v_\iota v_\iota^* =: P_\Lambda,$$

$$\Lambda := \{\lambda \in \sigma(A) : \lambda \in \Omega\}.$$

Discretization of the elliptic contour integral

Evaluation of the contour integral using the following equidistant parametrization of an elliptic contour centered at λ_0, with semiaxes R and r with N integration points

$$\begin{aligned}
\varphi_k &= \frac{2\pi}{N}(k - \frac{1}{2}), \quad k \in \{1, \ldots, N\},\\
z_k &= \lambda_0 + R\cos(\varphi_k) + \mathrm{i}r\sin(\varphi_k),\\
z'_k &= -R\sin(\varphi_k) + \mathrm{i}r\cos(\varphi_k),
\end{aligned}$$

yields using the composite trapezoidal rule:

$$\begin{aligned}
\frac{1}{2\pi\mathrm{i}}\int_{\partial\Omega}\frac{1}{z\mathbb{1} - A}dz &\approx \sum_{k=1}^{N}\omega_k\frac{1}{z_k\mathbb{1} - A},\\
\omega_k &= \frac{1}{\mathrm{i}N}z'_k.
\end{aligned}$$

Resolvent sampling

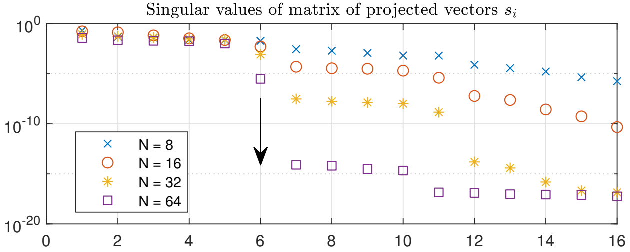
- Numerical problem: Evaluation of resolvent requires inverse
- Solution: Multiply $L > r$ random vectors y_i from the right on resolvent
- Corresponds to projecting L random vectors on approximated eigenspace

$$\frac{1}{z_k \mathbb{1} - A} y_i =: x_{ik},$$
$$(z_k \mathbb{1} - A) x_{ik} = y_i, \quad \Rightarrow \quad L \cdot N \text{ linear systems}$$

$s_i := \sum_k \omega_k x_{ik} \approx P_\Lambda y_i$ provides L vectors s_i that lie approximately in the desired eigenspace $\rightarrow$ Rayleigh–Ritz

Singular value decomposition and Rayleigh–Ritz

- L vectors s_i approximate an r-dimensional eigenspace
- Use a singular value decomposition to determine the dimension of the approximated eigenspace, to find out how many eigenvalues lie in the search domain
- gain the unitary vectors u_ι required for Rayleigh–Ritz



Reduction of linear systems: Moments and initial solution

Moments z^j help to create linear independent projected vectors on the approximated eigenspace:

$$\frac{1}{2\pi \mathrm{i}} \oint_{\partial\Omega} z^j \frac{1}{z\mathbb{1} - A} dz = \sum_{\lambda_\iota \in \Omega} \lambda_\iota^j v_\iota v_\iota^*.$$

Initializing x_{i1} to define $y_i := (z_1\mathbb{1} - A)x_{i1}$ saves L linear systems.

Rational interpolation method

Rational filter function:

$$H(z) = \frac{1}{\prod_k (z_k - z)} = \sum_k \frac{w_k}{z_k - z},$$

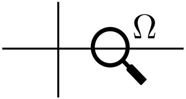
$$w_k = c \cdot \left(\prod_{j \neq k} (z_j - z_k) \right)^{-1}.$$

Amplification of projectors on eigenspace of eigenvalues λ_ι close to interpolation points z_k:

$$H(A) = \sum_k \frac{w_k}{z_k \mathbb{1} - A} = \sum_{\iota k} \frac{w_k}{z_k - \lambda_\iota} v_\iota v_\iota^*. \tag{1}$$

Program RESARARI, part 1

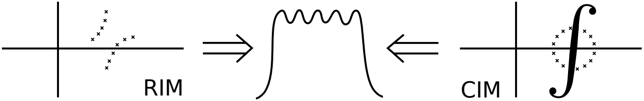
1) Search domain



Resolvent sampling Rayleigh-Ritz

2) Method

Rational filter function



Rational interpolation method

Contour integral method

3) Number of

Integration points	Moments	Random vectors for resolvent sampling
N	M	L

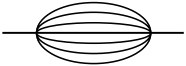
Program RESARARI, part 2

4) Discretization

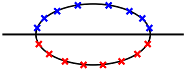
linear

chebyshev

eccentricity of ellipse



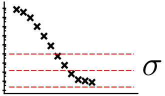
parametrization



5) Linear System

CHOOSE:
- solver
- preconditioner
- start vector
- max iterations
- symmetrized CIM
- accuracy of linear system solution

6) SVD Tolerance

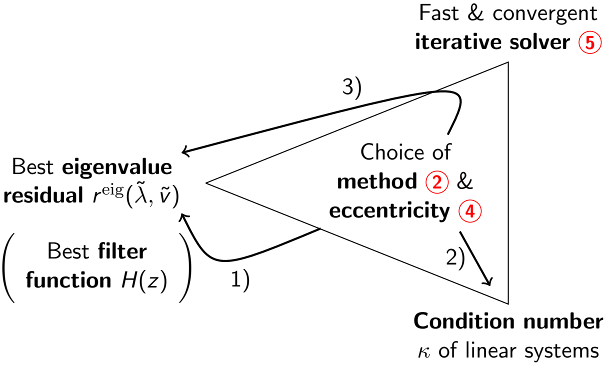


Result: $Av_i \approx \lambda_i v_i, \quad \lambda_i \in \Omega$

Research questions

Research questions:

1) Compare CIM (contour integral method) and RIM (rational interpolation method) in terms of filter functions
2) Analyze the condition number of the arising linear systems
3) Examine the influence of the accuracy of the solution of the linear systems (iterative solver) on the final residuals of the calculated eigenpairs



CIM versus RIM

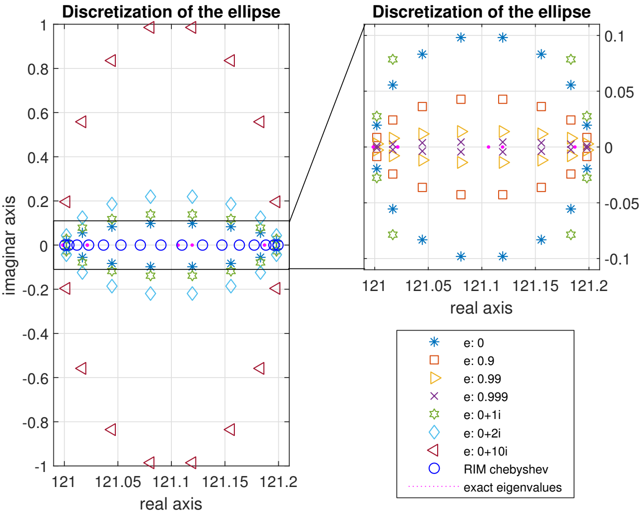
CIM

- $s_i = \sum_k \frac{\omega_k}{z_k \mathbb{1} - A} y_i$
- integration points z_k form a contour
- ω_k integration weights times Jacobian of parametrization

RIM

- $s_i = \sum_k \frac{w_k}{z_k \mathbb{1} - A} y_i$
- interpolation points z_k have to be close to domain of interest
- w_k barycentric weights of interpolation points

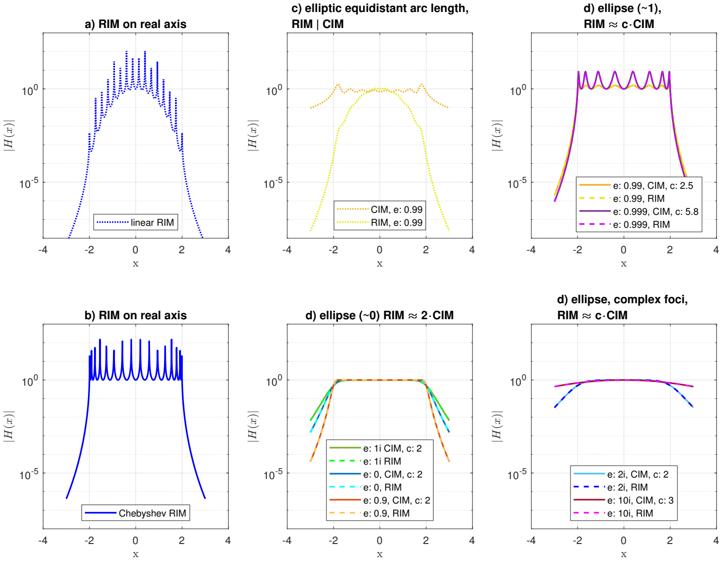
Different shapes (eccentricities) of the ellipse



Different parametrizations

a) equidistantly distributed along the real axis (linear RIM),
b) roots of the Chebyshev polynom as interpolation points on the real axis (Chebyshev RIM),
c) equidistantly distributed with respect to the arc length on an elliptic contour for different eccentricities (CIM and RIM),
d) uniformly distributed with respect to the parameter φ on an elliptic contour for different eccentricities (CIM and RIM).

Filter functions



Symmetrization of contour integral method

- Combine two linear systems to retrieve Hermitian linear system,
- Advantage: Hermitian and positive definite linear systems $\rightarrow$ conjugate gradient method
- Disadvantage: Condition number gets squared

SCIM in detail

Using the symmetry properties $\cos(\varphi_k) = \cos(\varphi_{N+1-k})$ and $\sin(\varphi_k) = -\sin(\varphi_{N+1-k})$, we have for $k = 1, \ldots, N/2$:

$$z_{N+1-k} = \overline{z_k}, \qquad z'_{N+1-k} = -\overline{z'_k},$$
$$\tilde{\omega}_{N+1-k} = \overline{\tilde{\omega}_k}, \qquad \omega_{N+1-k} = \overline{\omega_k},$$

$$S = \sum_{k=1}^{N/2} \left[\omega_k z_k^j \left(z_k \mathbb{1} - A\right)^{-1} - \overline{\omega_k z_k}^j \left(\overline{z_k}\mathbb{1} - A\right)^{-1}\right] Y =$$
$$= \sum_{k=1}^{N/2} \underbrace{\left[\omega_k z_k^j (\overline{z_k}\mathbb{1} - A) - \overline{\omega_k z_k}^j (z_k \mathbb{1} - A)\right]}_{=:\omega_{kj}} \left[\underbrace{(z_k \mathbb{1} - A)(\overline{z_k}\mathbb{1} - A)}_{=:\tilde{A}_k}\right]^{-1} Y.$$

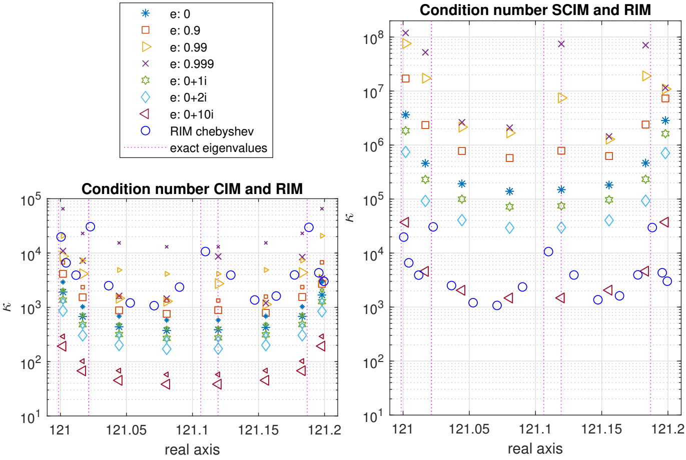
Positive definite linear system

By decomposing the discretization points in real and imaginary parts $z_k = z_k^{(\mathrm{r})} + \mathrm{i} z_k^{(\mathrm{i})}$, the matrix can be written as:

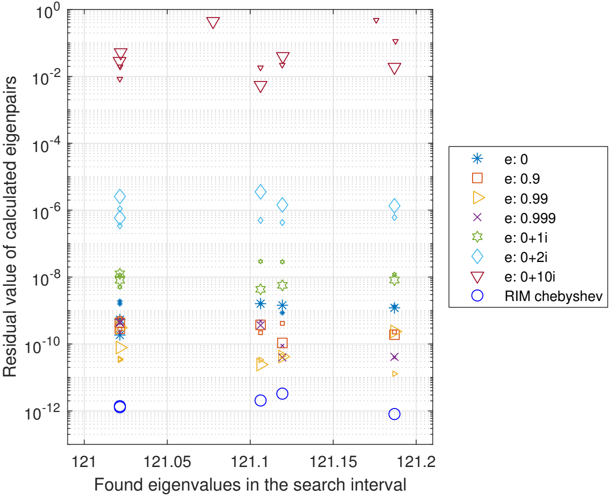
$$\begin{aligned}\tilde{A}_k &= (z_k^{(\mathrm{r})}\mathbb{1} - A + z_k^{(\mathrm{i})})(z_k^{(\mathrm{r})}\mathbb{1} - A - z_k^{(\mathrm{i})}) \\ &= (z_k^{(\mathrm{r})}\mathbb{1} - A)^2 + {z_k^{(\mathrm{i})}}^2\mathbb{1}.\end{aligned}$$

- If $z_k^{(\mathrm{i})} \neq 0$, linear system is positive definite.

Condition number comparison



Eigenproblem residual for different methods using direct solver (Matlab)



(Reached relative linear residual of the order of 10^{-13}.)

Used iterative solvers and parameters

1. GMRES(20) for CIM,
2. BiCGSTAB for CIM,
3. MINRES for RIM,
4. SYMMLQ for RIM,
5. PCG for SCIM.

Fixed parameters for the iterative solvers:

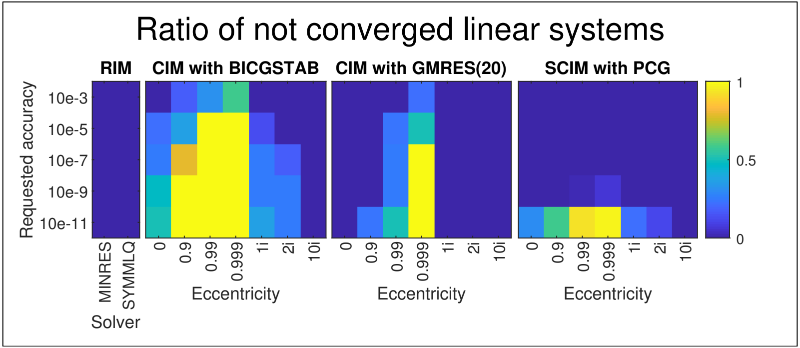
- maximum number of iterations $\texttt{maxit} = 8000$
- discretization points $N = 16$
- random vectors $L = 16$
- moments $M = 4$
- start vector x_0 equal to the previous solution

Accuracy of the solution $x^{(m)}$ of the linear system $Ax = y$ after m iteration steps measured by the relative residual r^{lin}:

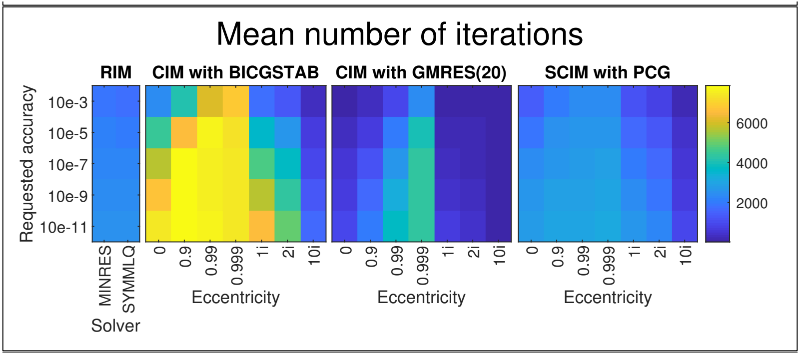
$$r^{\mathrm{lin}}(x^{(m)}) = \frac{\|Ax^{(m)} - y\|}{\|y\|}.$$

Criteria to examine the performance of the iterative solver in the context of the eigensolver

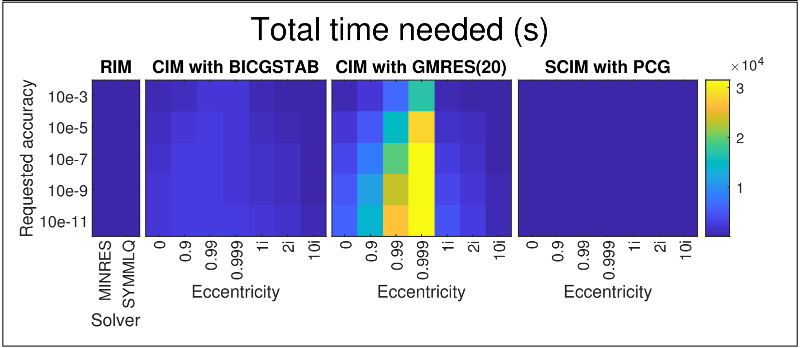
1. Percentage of not converged linear systems,
2. Mean number of iterations needed,
3. Total time for the calculation,
4. Mean reached relative residual r^{lin} of the solution $x^{(m)}$ of the linear systems,
5. Number of found eigenvalues in the domain (should be five),
6. Mean eigenvalue residual r^{eig} of the five best solutions,



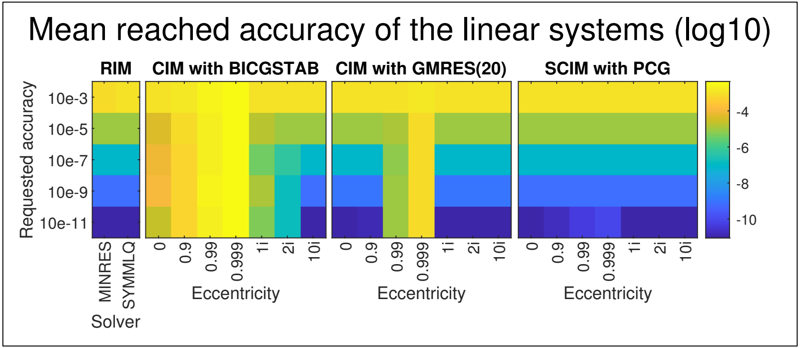
- BICGSTAB and GMRES rather bad



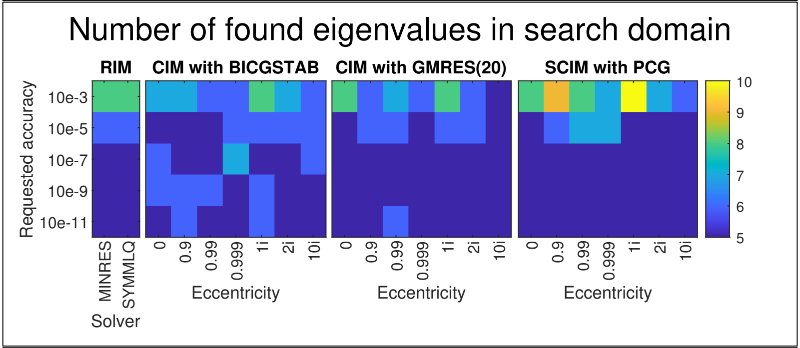
- BICGSTAB ran into maximum number of iterations

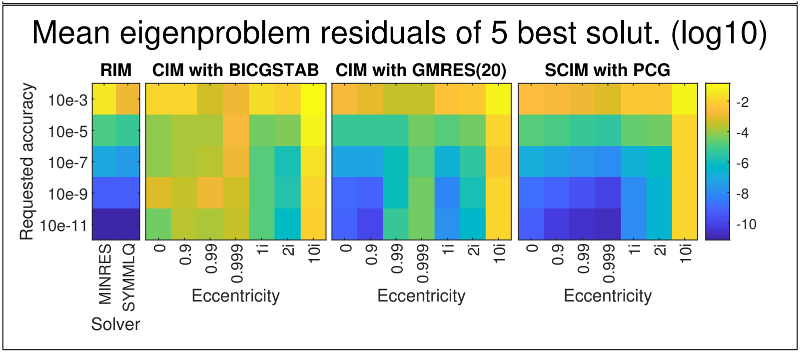


- GMRES took most of the time (restarted GMRES after 20 iterations)



- reflects convergence of iterative solvers


Number of found eigenvalues in search domain
RIM
CIM with BICGSTAB
CIM with GMRES(20)
SCIM with PCG
Requested accuracy
10e-3
10e-5
10e-7
10e-9
10e-11
MINRES
SYMMLQ
Solver
0
0.9
0.99
0.999
1i
2i
10i
Eccentricity
10
9
8
7
6
5



- RIM and SCIM perform well for the chosen iterative solvers.

Findings from research question 1: comparison RIM and CIM

1. Quality of eigenspace projector can be analyzed and compared in terms of filter functions.
2. The absolute value of the filter functions $H(z)$ derived from Chebyshev RIM and uniform parameter CIM are identical up to a constant factor c
3. Chebyshev nodes (RIM) and uniformly distributed parameter discretization points (CIM) have the same real parts and coincide for an eccentricity going to one. Both show a rather homogeneous filter function behavior.
4. Linear nodes (RIM) and equidistant arc length discretization points (CIM) lead to inhomogeneous filter functions that amplify mostly the center of the search domain.

Findings from research question 2: SCIM and condition number

1. The condition number becomes worse when using eccentricities close to one (small semi-minor axis) and rather small for large complex eccentricities (large semi-minor axis).
2. The symmetrized contour integral method (SCIM) yields positive definite linear systems which have a quadraticly worse condition number than linear systems obtained from using CIM.
3. The condition number of RIM is roughly in between those resulting from CIM and SCIM.

Findings from research question 3a: direct solver and shape of the contour

1. The larger the semi–minor axis within CIM and SCIM the worse the reached accuracy of eigenvalues. This can be understood from the shape of the filter functions.
2. CIM and SCIM yield approximately the same reached accuracy of eigenvalues (eigenvalue residual r^{eig}) depending on the eccentricity e when using a direct solver.
3. SCIM has the advantage of halving the number of linear systems to solve compared to CIM.

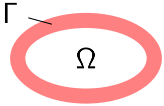
Findings from research question 3b: iterative solver and reached accuracy of the solution of the eigenproblem

1. BICGSTAB and GMRES show convergence issues.
2. RIM in combination with SYMMLQ or MINRES shows the best results in terms of reached final eigenvalue residuals and total time needed.
3. SCIM in combination with PCG can achieve results comparable with RIM provided the used contour has a small semi–minor axis (eccentricity close to one).
4. CIM in combination with GMRES can be used to obtain moderate results provided that the semi–minor axis is not too small otherwise convergence issues arise.
5. All-in-all it is best to deal with symmetric linear systems when dealing with iterative solvers even on the cost of an increasing condition number.

Outlook

1. Krylov space recycling
2. Preconditioning
3. Successive improvements of the eigensolution
   - Adding new sampling points z_k,
   - Adding new moments z_k^j,
   - Adding new right hand sides y_i,
   - Iterate on the solution of linear systems.
4. Idea to improve the filter function not only by amplification but by suppressing the surrounding (inspired by STED - Stimulated Emission Depletion)

$$H(z) = \left(\prod_{k, z_k \in \Omega} z_k - z \right)^{-1} \prod_{j, z_j \in \Gamma} (z_j - z)$$



Literature

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