The FEAST Algorithm for Sparse Symmetric Eigenvalue Problems

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Problem statement

- FEAST algorithm: find all eigenpairs $(\lambda, \mathbf{x})$ of a real symmetric matrix $\mathbf{A}$ with
$$\lambda \in [\lambda_-, \lambda_+] =: \mathcal{L}.$$
- Our focus: $\mathbf{A}$ is large and sparse
  - FEAST involves linear system solves – want to use iterative solvers

FEAST overview

Subspace iteration

Pick p random n-vectors

$$\mathbf{Q}_{(0)} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \dots, \boldsymbol{q}_p]$$

For $k = 1,2, \dots$

$\tilde{\mathbf{Y}}_{(k)} \leftarrow \mathbf{A} \cdot \mathbf{Q}_{(k-1)}$

Orthonormalize $\tilde{\mathbf{Y}}_{(k)}$ into $\mathbf{Y}_{(k)}$

Form $p \times p$ system $\widehat{\mathbf{A}} = \mathbf{Y}_{(k)}^H \mathbf{A} \mathbf{Y}_{(k)}$

Compute eigenpairs $(\hat{\lambda}, \widehat{\mathbf{X}})$ of $\widehat{\mathbf{A}}$

$\mathbf{Q}_{(k)} \leftarrow \mathbf{Y}_{(k)} \widehat{\mathbf{X}}$

$\mathbf{Q}_{(k)}$: converges linearly to the p dominant eigenvectors of $\mathbf{A}$ (convergence factor to eigenvector i: $|\lambda_{p+1}/\lambda_i|$)

FEAST overview

Subspace iteration + filtering

Pick p random n-vectors

$$\mathbf{Q}_{(0)} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \dots, \boldsymbol{q}_p]$$

For $k = 1,2,\dots$

$\tilde{\mathbf{Y}}_{(k)} \leftarrow \rho(\mathbf{A}) \cdot \mathbf{Q}_{(k-1)}$

Orthonormalize $\tilde{\mathbf{Y}}_{(k)}$ into $\mathbf{Y}_{(k)}$

Form $p \times p$ system $\widehat{\mathbf{A}} = \mathbf{Y}_{(k)}^H \mathbf{A} \mathbf{Y}_{(k)}$

Compute eigenpairs $(\hat{\lambda}, \widehat{\mathbf{X}})$ of $\widehat{\mathbf{A}}$

$\mathbf{Q}_{(k)} \leftarrow \mathbf{Y}_{(k)} \widehat{\mathbf{X}}$

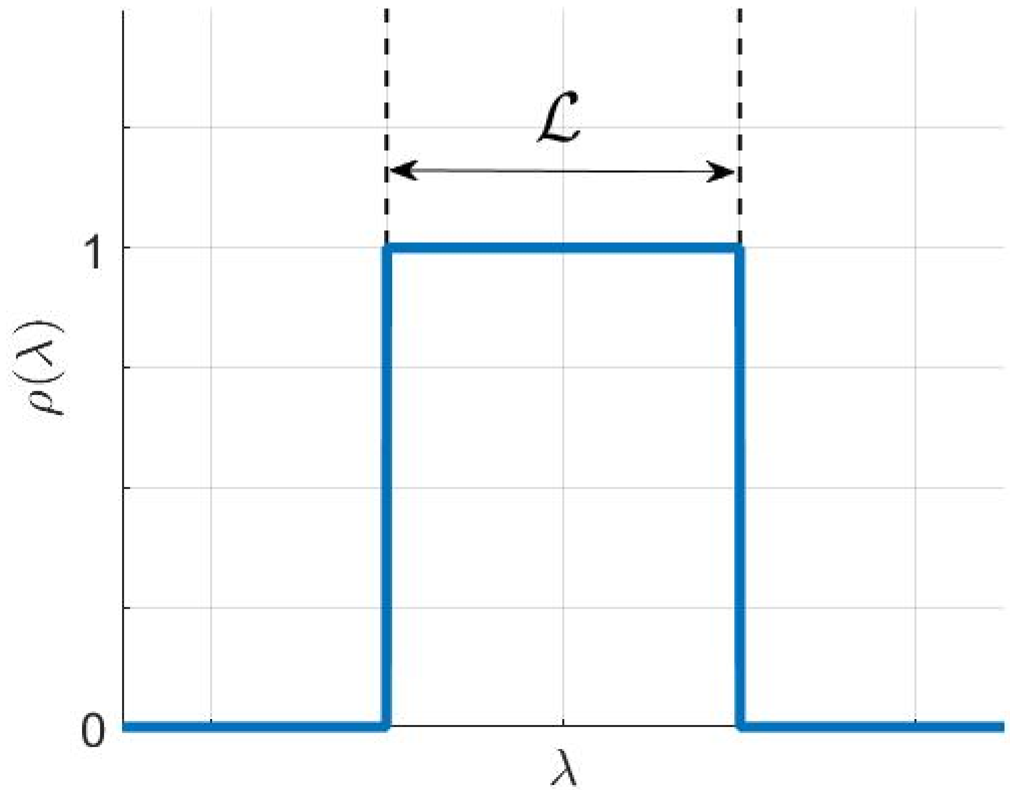
…where $\rho(\mathbf{A})$ preserves eigenvectors and maps eigenvalues λ to $\rho(\lambda)$.

$\mathbf{Q}_{(k)}$: converges linearly to the p dominant eigenvectors of $\rho(\mathbf{A})$ (convergence factors: $|\rho(\lambda_{p+1})/\rho(\lambda_i)|$)

Examples:

- $\rho(\mathbf{A}) = \mathbf{A}^k$
  $\rightarrow \rho(\lambda) = \lambda^k$
- $\rho(\mathbf{A}) = (\mathbf{A} - \sigma \mathbf{I})^{-1}$
  $$\rightarrow \rho(\lambda) = \frac{1}{\lambda - \sigma}$$

FEAST overview: choice of filter



Ideal: indicator function over $\mathcal{L}$

$$\rho(\mathbf{A}) = ???$$

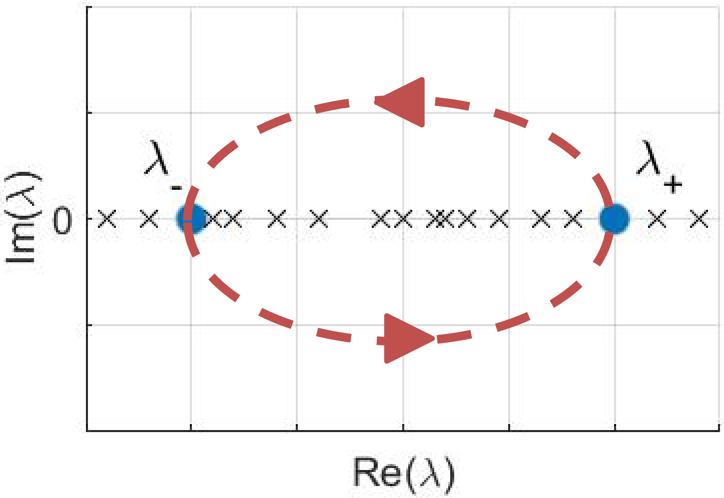
FEAST overview: choice of filter

Cauchy's Integral Theorem

Let Γ be a contour in the complex plane. Then the (counter-clockwise) contour integral

$$\pi(\lambda) = \frac{1}{2\pi\imath}\oint_\Gamma \frac{1}{z-\lambda}\,\mathrm{d}z\,, \qquad \lambda \notin \Gamma$$

is equal to 1 for λ enclosed in Γ, and 0 for λ not enclosed in Γ.

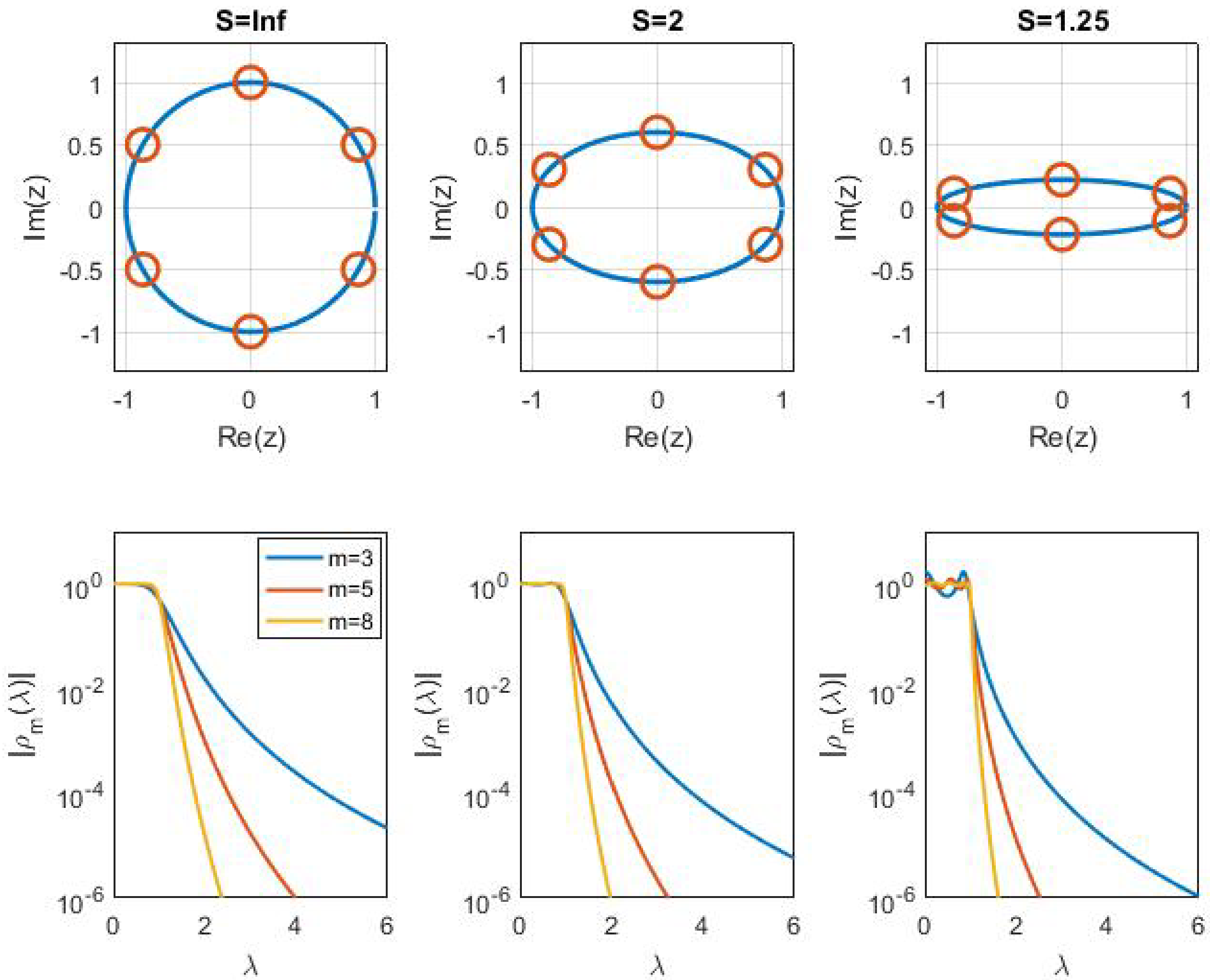


k-point quadrature $\Rightarrow$

$$\pi(\lambda) \approx \rho(\lambda) := \sum_{i=1}^{k} \frac{w_i}{z_i - \lambda}$$

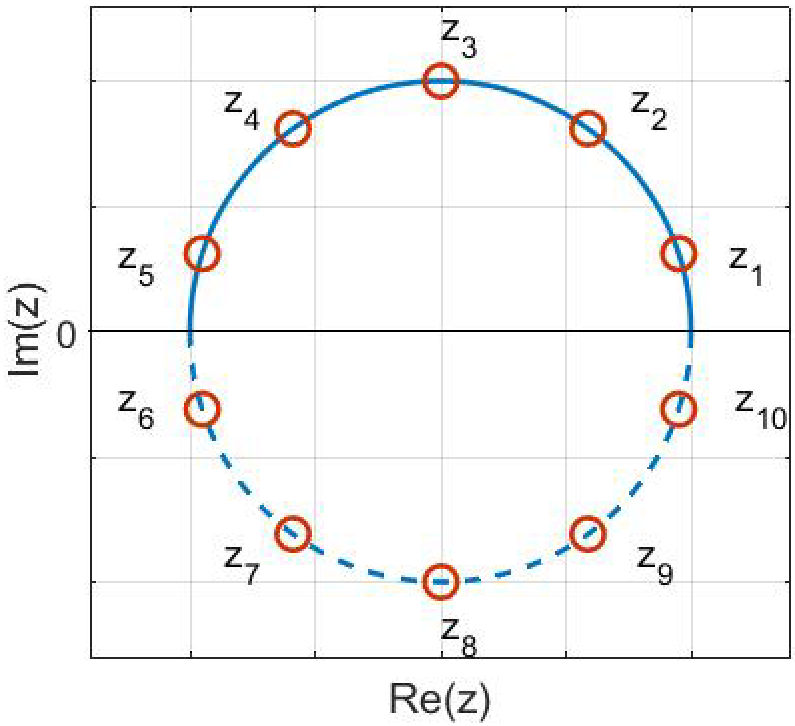
$$\rho(\mathbf{A}) := \sum_{i=1}^{k} w_i (z_i \mathbf{I} - \mathbf{A})^{-1}$$

Trapezoidal rule



On $[-1,1]$ for different (half) number of nodes m

Computing $\rho(\mathbf{A})\mathbf{Q}$



Trapezoidal quadrature points
$S = \infty, m = 5$

- For $\mathbf{Q} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \dots, \boldsymbol{q}_p]$,
  $\rho(\mathbf{A})\mathbf{Q} = \sum_{i=1}^{2m} w_i (z_i \mathbf{I} - \mathbf{A})^{-1} \mathbf{Q}$
- **Note:** nodes z are in complex conjugate pairs
- For real $\mathbf{A}, \mathbf{Q}$:
  $(\bar{z}\mathbf{I} - \mathbf{A})^{-1}\mathbf{Q} = \overline{(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{Q}}$
- Therefore: in real case, only need to solve mp linear systems to compute $\rho(\mathbf{A})\mathbf{Q}$ (instead of $2mp$)

Computing $\rho(\mathbf{A})\mathbf{Q}$

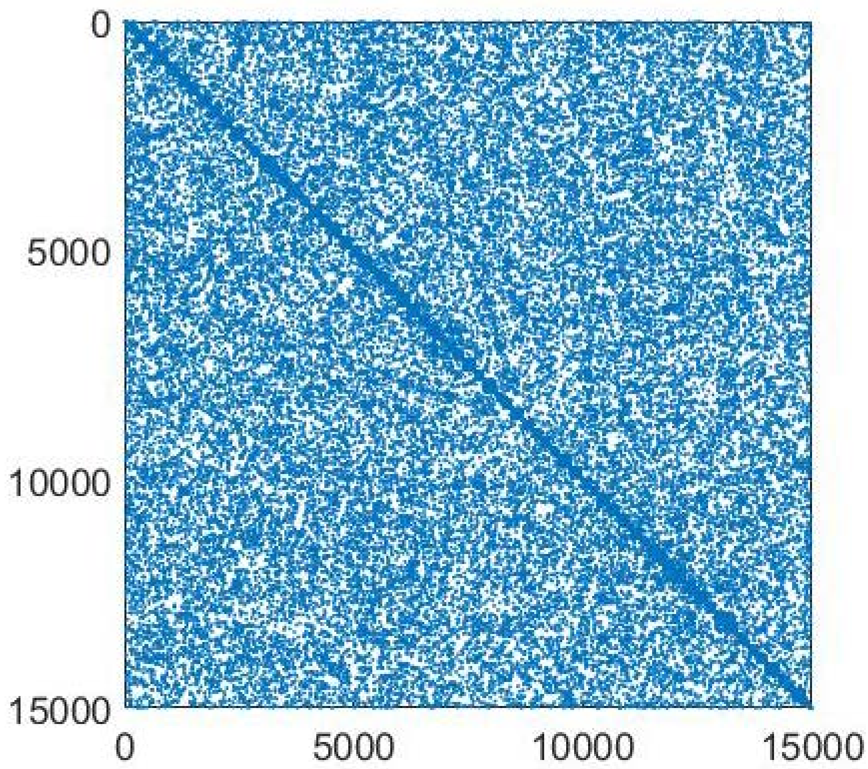
At each FEAST iteration: solve mp linear systems
$$(z_i\mathbf{I} - \mathbf{A})\boldsymbol{y}_{i,j} = \boldsymbol{q}_j, \qquad 1 \leq i \leq m, 1 \leq j \leq p.$$

- Usual approach in FEAST literature: use direct solvers
  - What if $\mathbf{A}$ is large and sparse?
  - …or we don't need highly accurate solutions?
- Our goal: use iterative solvers instead
  - Some challenges:
    - Systems are indefinite, non-Hermitian (even for Hermitian $\mathbf{A}$)
    - Conditioning issues
    - Lots of right-hand sides

Numerical experiments

- Direct solvers vs. preconditioned GMRES
- Two matrices: finding 100 eigenpairs of each (with search space size $p = 130$)
- FEAST tolerance: 10^{-10}
- Quadrature: $S = 1.05,\ m = 8$
- Coded in MATLAB

Matrix 1: Andrews



$n = 60{,}000;\ nnz = 760{,}154$

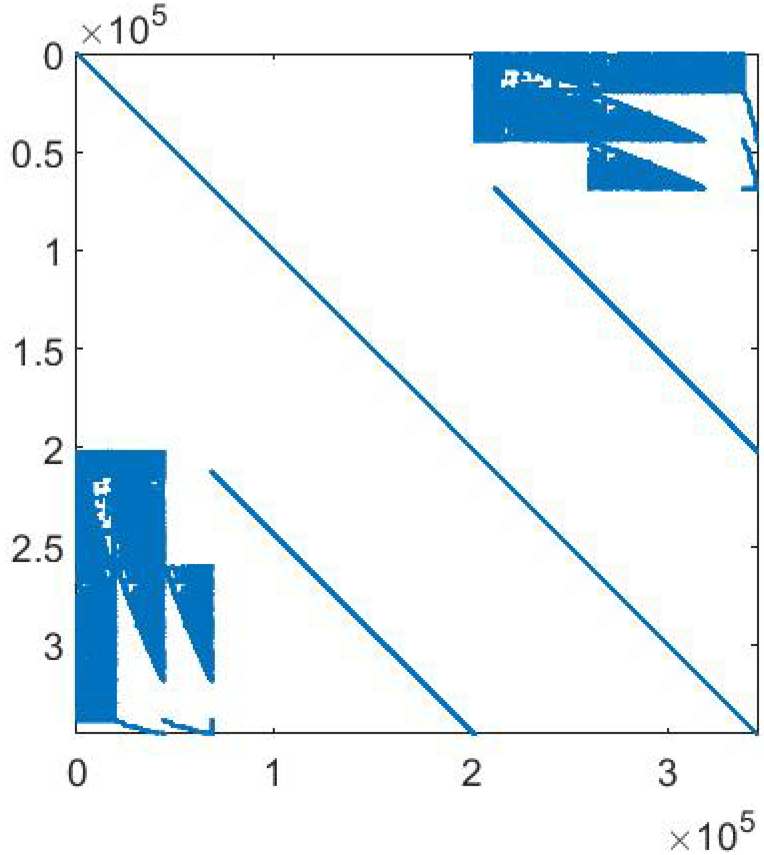
- $[\lambda_-, \lambda_+] = [0.0, 1.3]$ (100 smallest)
- GMRES solver:
  - Tolerance: 10^{-10}
  - Preconditioner: ILUTP ($\tau = 5.0 \times 10^{-3}$)
- Direct solver: backslash

Andrews matrix results

	GMRES with ILUTP	Direct solver
$nnz(L+U)$ (average over all shifted systems)	2,767,412	234,019,880
FEAST iterations to convergence	3	3
Average time per LS solve	7.9 s (119.0 iterations)	2.0 s
Total time	26,462 s*	6,530 s

*= includes time for preconditioner construction

Matrix 2: c-big



$n = 345{,}241$; $nnz = 2{,}340{,}859$

- $[\lambda_-, \lambda_+] = [45.2, 50.0]$ (interior)
- GMRES solver:
  - Tolerance: 10^{-10}
  - Preconditioner: ILUTP ($\tau = 1.0 \times 10^{-3}$)

c-big results

	GMRES with ILUTP	Direct solver
$nnz(L+U)$ (average over all shifted systems)	5,697,775	144,569,235
FEAST iterations to convergence	3	3
Average time per LS solve	2.5 s (8.5 iterations)	1.6 s
Total time	7,795 s*	4,979 s

*= includes time for preconditioner construction

Discussion/considerations

- Speed vs. memory
  - On our 60k matrix – per linear system: iterative solver takes 4x the time, ~1/25th of the memory
  - On 345k: 1.6x the time, ~1/17th of the memory
- Direct solver loses a level of parallelism
  - Can overcome this (to an extent) with a different direct solver
- Lots of improvements to explore for the iterative solvers…

Future work

- Krylov space recycling
- Preconditioned MINRES
- More parallelization
- Generalized and non-Hermitian problems

Thank you

- Chen
- Robert and Uri
- Ian
- Audience