Control of the search space size and solving linear systems in the FEAST algorithm

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Joint work with

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http://www.sppexa.de
http://blogs.fau.de/essex/

Outline

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Symmetric eigenvalue problem

We aim at solving the problem:

Given: $\mathsf{A} \in \mathbb{R}^{n\times n},\ \mathsf{A} = \mathsf{A}^\star$,
an interval

$$I_\lambda = [\,\underline{\lambda},\, \overline{\lambda}\,]\,.$$

Sought: $\mathsf{X} \in \mathbb{R}^{n\times m}$, $m \leq n$, $\mathsf{X}^\star\mathsf{X} = \mathsf{I}$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$ such that

$$\mathsf{AX} = \mathsf{X}\Lambda \text{ and all } \lambda_j \in [\underline{\lambda},\, \overline{\lambda}]\,.$$

✎ Solve the (partial) symmetric eigenproblem. Find all eigenvalues in a given interval.

(Everything can be generalized to complex matrices and to a pair (A, B) with B hpd.)

Framework: Rayleigh-Ritz approach

- Choose a subspace $\mathcal{U} = \mathrm{span}(\mathsf{U}), \mathsf{U} \in \mathbb{C}^{n \times m}$.
- Compute the Rayleigh quotients $\mathsf{A}_\mathsf{U} := \mathsf{U}^\star \mathsf{A} \mathsf{U},\ \mathsf{B}_\mathsf{U} := \mathsf{U}^\star \mathsf{B} \mathsf{U}$.

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- Compute eigenpairs $(\widetilde{\Lambda}, \widetilde{\mathsf{W}})$ of $\mathsf{A}_\mathsf{U} \mathsf{W} = \mathsf{B}_\mathsf{U} \mathsf{W} \Lambda$.
- Form Ritz pairs $(\widetilde{\Lambda}, \mathsf{U}\widetilde{\mathsf{W}})$ of $\mathsf{A}\mathsf{X} = \mathsf{B}\mathsf{X}\Lambda$.

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- Form Ritz pairs $(\widetilde{\Lambda}, \mathsf{U}\widetilde{\mathsf{W}})$ of $\mathsf{A}\mathsf{X} = \mathsf{B}\mathsf{X}\Lambda$.

...and hope that $(\widetilde{\Lambda}, \mathsf{U}\widetilde{\mathsf{W}})$ are good approximations to some eigenpairs.
Otherwise, set $\mathsf{U} := \mathsf{U}\widetilde{\mathsf{W}}$ and iterate.

The subspace in use

E. Polizzi, Phys. Rev. B, 2009, 79, 115112

In FEAST: The subspace

$$U := \frac{1}{2\pi\imath}\int_{\mathcal{C}} (zB - A)^{-1} \mathrm{d}z BY$$

is used.

- $\mathcal{C}$ = curve in complex plane surrounding I_λ.
- Y = starting base of (possibly) random vectors.

It follows

$$\frac{1}{2\pi\imath}\int_{\mathcal{C}} (zB - A)^{-1} B \mathrm{d}z = \text{orth. projector onto} \quad \mathrm{span}(X)$$

The FEAST Algorithm: Skeleton

Input: $I_\lambda := [\underline{\lambda}, \overline{\lambda}]$, an estimate $\widetilde{m}$ of the number of eigenvalues in I_λ.

Output $\hat{m} \leq \widetilde{m}$ eigenpairs with eigenvalue in I_λ.

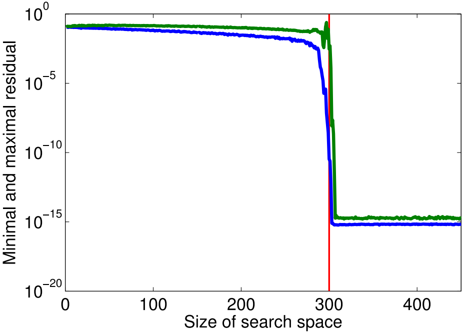
Perform:

1. Choose $\mathsf{Y} \in \mathbb{C}^{n \times \widetilde{m}}$ of full rank and compute $\mathsf{U} := \frac{1}{2\pi \mathbf{i}} \int_{\mathcal{C}} (z\mathsf{B} - \mathsf{A})^{-1} \mathsf{B} \, \mathrm{d}z \, \mathsf{Y}$,
2. Form $\mathsf{A}_\mathsf{U} := \mathsf{U}^\star \mathsf{A} \mathsf{U}, \ \mathsf{B}_\mathsf{U} := \mathsf{U}^\star \mathsf{B} \mathsf{U}$,
3. Solve size-$\widetilde{m}$ eigenproblem $\mathsf{A}_\mathsf{U} \widetilde{\mathsf{W}} = \mathsf{B}_\mathsf{U} \widetilde{\mathsf{W}} \widetilde{\Lambda}$,
4. Compute $(\widetilde{\Lambda}, \widetilde{\mathsf{X}} := \mathsf{U} \cdot \widetilde{\mathsf{W}})$,
5. If no convergence: go to Step 1 with $\mathsf{Y} := \widetilde{\mathsf{X}}$.

Problem: How to choose search space size $\widetilde{m}$?

Experiment: Choose $I_\lambda = [\underline{\lambda}, \overline{\lambda}]$ such that it contains the $m = 300$ lowest eigenvalues of size 1059-matrix. Let $\widetilde{m}$ vary, $\widetilde{m} = 1, \ldots, 450$.

Residuals vs. search space size $\widetilde{m}$:



K., Di Napoli, Galgon, Lang, Bientinesi: *Dissecting the FEAST algorithm for generalized eigenproblems*, 2013

Problem: How to choose search space size $\widetilde{m}$?

Do not choose too small!

$$\text{Determine a good choice for } \widetilde{m} \Leftrightarrow \text{Count eigenvalues in } I_\lambda$$

Leads to stopping criterion:

$$\text{“all” eigenpairs found} \Rightarrow \text{Stop Algorithm}$$

Counting eigenvalues

- $\mathrm{rank}(U) = m =$ number of eigenvalues in I_λ
- In exact arithmetic: U has singular values 0 or 1
- numerical rank?

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- $\mathrm{rank}(U) = m =$ number of eigenvalues in I_λ
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- numerical rank?
- It can be shown: If $m \leq \widetilde{m}$ we have $m = \#$ of singular values of U that are $\geq 1/2$ (Tang & Polizzi, 2013).
- Number $1/2$ depends on implementation (integration scheme). E.g., valid for Gauß–Legendre integration, midpoint rule of even order.

Counting eigenvalues: SVD of U

SVD $\mathsf{U} = \mathsf{W}\Sigma\mathsf{V}^\star$ with $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_m, 0, \ldots, 0)$

$\Rightarrow$ $\mathrm{span}(\mathsf{W}(:, 1:m)) = \mathrm{span}(\mathsf{U})$

$\Rightarrow$ Found the correct subspace, but cost $= \mathcal{O}(n^2 \cdot \widetilde{m})$

SVD of $\mathsf{B}_\mathsf{U} = \mathsf{U}^\star\mathsf{B}\mathsf{U}$:

$\Rightarrow$ $\mathsf{B}_\mathsf{U} = \mathsf{V}\Sigma^\star\Sigma\mathsf{V}^\star$ with $\mathsf{V} \in \mathbb{R}^{\widetilde{m}\times\widetilde{m}}$, orthogonal. No order n cost.

$\Rightarrow$ $\mathsf{U}' = \mathsf{U} \cdot \mathsf{V}(:, 1:m)$ spans the wanted space $\rightsquigarrow \mathcal{O}(n \cdot m)$.

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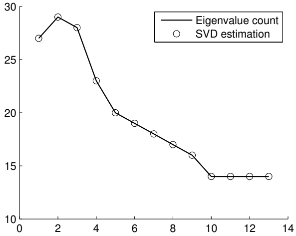
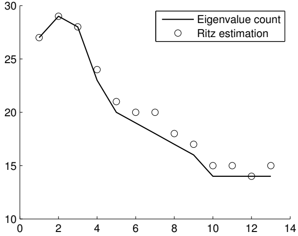
This means the dimension and a basis of the search space can be computed.

Proceed with a subspace slightly larger than m.

SVD count



Number of Ritz values in I_λ



1 Point on abscissa $\equiv$ 1 interval I_λ

$\circ =$ count from respective method

line $=$ exact count

✎ Ritz count is almost for free and not too bad. It does not deliver the subspace. Typically overestimates.

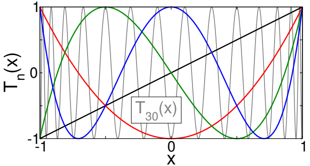
Counting eigenvalues: alternatives

Chebyshev polynomials

two-term recurrence

$$T_n(x) = \cos(n \arccos x)$$

$$T_0(x) = 1\ , \quad T_1(x) = x\ ,$$
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$



Expansion of functions

for example: density of states (DOS) $\hat{=}$ eigenvalue count

$$\rho(\omega) \propto \mu_0 + 2\sum_{n=1} \mu_n T_n(\omega)$$

with coefficients (moments) of the matrix A

$$\mu_n = \int_{-1}^{1} \rho(\omega)\, T_n(\omega)\, \mathrm{d}\omega$$
$$= \mathsf{x}^\star T_n(\mathsf{A})\mathsf{x}$$

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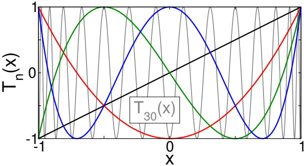


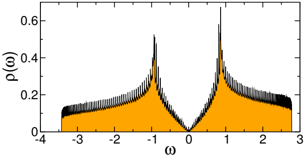
Expansion of functions

for example: density of states (DOS) $\hat{=}$ eigenvalue count

idea: use as input for FEAST

further technical details: Weiße, Wellein, Alvermann, Fehske, Rev. Mod. Phys. 78, 275 (2006).

cf. recent report (Di Napoli *et al.*, 2013)



Outline

Linear systems

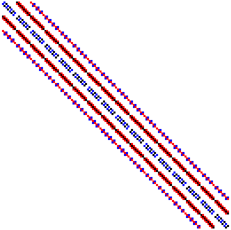
Central task: Solution of

$$(z\mathsf{B} - \mathsf{A})\mathsf{V} = \mathsf{B}\mathsf{Y}.$$

Matrix $(z\mathsf{B} - \mathsf{A})$ is

- large and sparse ~~Cholesky~~ ~~LU~~
- non-Hermitian (z complex) ~~Cholesky~~ ~~CG~~
- complex valued
- often ill-conditioned ~~GMRES~~ GMRES??

Problems from Graphene nanoribbons



some lead to banded systems ⇒ special banded direct solver.
See (Hockney & Jesshope, 1988) and (Lawrie & Sameh, 1984).

Results with banded solver

- Matrix size $n \approx 1.2M$, ratio $\frac{\text{nnz}}{n^2} \approx 0.001\%$ (12 nonzero entries per row).
- Graphene II with gap around zero.

Matrix	est.	found	iters.
Graphene I	535	535	7
Graphene II (ℓ)	492	492	4
Graphene II (r)	546	546	8
Graphene III	574	572	25

- Eigenpair residuals: $10^{-9} \dots 10^{-16}$
- Linear system residuals: $10^{-10} \dots 10^{-16}$

General (non-banded) problems

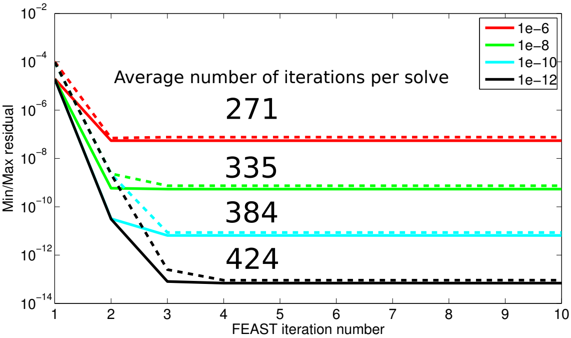
Problem large & sparse: Iterative method needed.
Candidate 1: Special tailored method for systems

$$(\mathsf{R} + \mathbf{i}\mathsf{S})(\mathsf{x} + \mathbf{i}\mathsf{y}) = \varphi + \mathbf{i}\psi$$
$$\mathsf{R} = \mathsf{R}^T, \mathsf{S} = \mathsf{S}^T, \text{ real}$$

(Axelsson & Kucherov, 2000)

- $(z\mathsf{B} - \mathsf{A})\mathsf{V} = \mathsf{BY}$ can be brought to this form.
- Leads to real systems of size $2n$.
- Not efficient enough in practice

Problem large & sparse: Iterative method needed.
Candidate 2: CARP-CG
(cf. Talk of Jonas Thies, Code also by Jonas)
Experiment: Graphene, $n = 4{,}200$, $m = 17$ interior eigenpairs
Achievable residuals $\|\mathsf{A}\mathsf{x} - \mathsf{x}\lambda\|$:



$$\max_{z_j} \kappa(z_j \mathsf{I} - \mathsf{A}) = 1097.$$

Larger example

Example 1: Graphene, $n = 84{,}000$, sought $m = 102$ eigenpairs from interior.

Average: 567 iterations/solve.

- $\mathrm{tol}_{\mathrm{lin}} = 10^{-10}$
- $\|\mathsf{A}\mathsf{x} - \mathsf{x}\lambda\| = 10^{-7} \ldots 10^{-10}$ (convergence criterion: 10^{-7}).
- Orthogonality $\max_{i \neq j} |\mathsf{x}_i^\star \mathsf{x}_j| = 10^{-15}$.

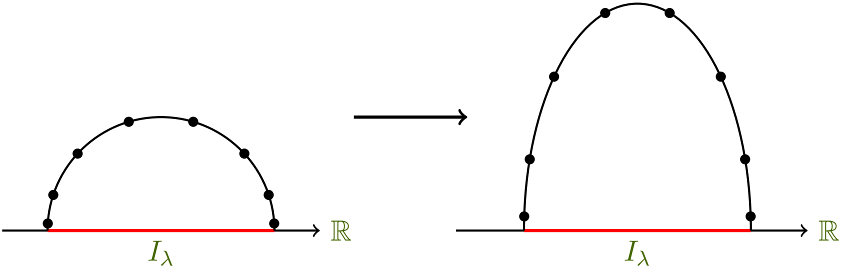
Example 2: Graphene, $n = 176{,}000$, sought $m = 201$ eigenpairs from interior.

Average: 655 iterations/solve.

- $\mathrm{tol}_{\mathrm{lin}} = 10^{-10}$
- $\|\mathsf{A}\mathsf{x} - \mathsf{x}\lambda\| = 10^{-8} \ldots 10^{-10}$ (convergence criterion: 10^{-7}).
- Orthogonality $\max_{i \neq j} |\mathsf{x}_i^\star \mathsf{x}_j| = 10^{-15}$.

Other contours

Idea: Bring integration points away from real axis.

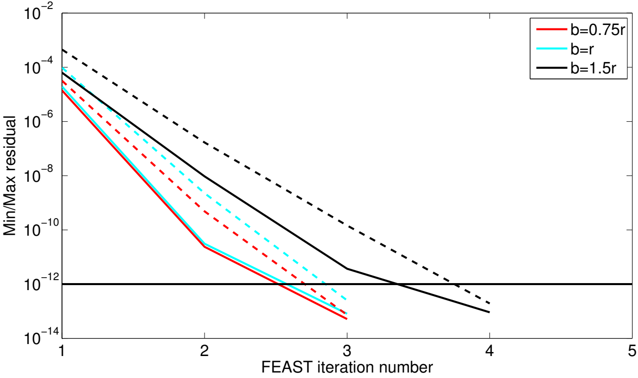


Use $\mathsf{U} = \frac{1}{2\pi\mathbf{i}}\mathsf{A}\int_{\mathcal{C}} \frac{1}{z}(z\mathsf{I} - \mathsf{A})^{-1}\mathrm{d}z$

Use of ellipse: Results

Experiment: Graphene, $n = 4{,}200$, $m = 17$ interior eigenpairs

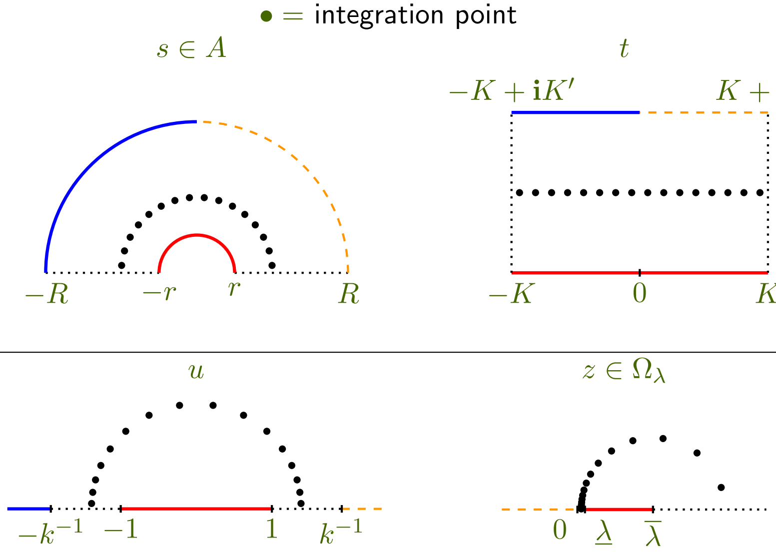
$r =$ main semi axis, second semi axis $b = \alpha r$, vary α



Required $\|Ax - x\lambda\| \leq 10^{-12}$.

$\Downarrow$ CARP-CG iterations $\leftrightarrow$ FEAST iterations $\Uparrow$

Outline



● = integration point
$s \in A$
$-R$
$-r$
r
R
t
$-K + \mathbf{i}K'$
$K + \mathbf{i}K'$
$-K$
0
K
u
$-k^{-1}$
-1
1
k^{-1}
$z \in \Omega_\lambda$
0
$\underline{\lambda}$
$\overline{\lambda}$

Outlook: Transforming the integration region

... for computing upper eigenpairs

Adapted from (Hale *et al.*, 2008): results in

$$\mathsf{U} = -\frac{\sqrt{\underline{\lambda}\overline{\lambda}}}{\pi \mathbf{i} k} \int_{-K+\mathbf{i}K'/2}^{3K+\mathbf{i}K'/2} \frac{\mathrm{cn}(t)\mathrm{dn}(t)}{(k^{-1} - \mathrm{sn}(t))^2} (z(t)\mathsf{B} - \mathsf{A})^{-1} \mathsf{B} \mathrm{d}t \mathsf{Y},$$

with $k = \frac{\sqrt{\overline{\lambda}/\underline{\lambda}}-1}{\sqrt{\overline{\lambda}/\underline{\lambda}}+1} < 1$. Then use midpoint rule.

Outlook: Transforming the integration region

... for computing upper eigenpairs

Adapted from (Hale *et al.*, 2008): results in

$$\mathsf{U} = -\frac{\sqrt{\underline{\lambda}\overline{\lambda}}}{\pi \mathbf{i} k} \int_{-K+\mathbf{i}K'/2}^{3K+\mathbf{i}K'/2} \frac{\mathrm{cn}(t)\mathrm{dn}(t)}{(k^{-1} - \mathrm{sn}(t))^2} (z(t)\mathsf{B} - \mathsf{A})^{-1} \mathsf{B} \mathrm{d}t \mathsf{Y},$$

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Theorem: (Hale *et al.*, 2008)

Let A, B *be real symmetric and let* $I_\lambda = [\underline{\lambda}, \overline{\lambda}] \subset (0, +\infty)$, *let* $\widetilde{\mathsf{U}}_p$ *formed by midpoint rule, then for all* $\underline{\lambda}, \overline{\lambda} > 0$

$$\|\mathsf{U} - \widetilde{\mathsf{U}}_p\| = \mathcal{O}\left(\exp\left(\frac{-\pi^2 p}{\log(\overline{\lambda}/\underline{\lambda}) + 3}\right)\right).$$

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$\mathcal{O}\left(\log\left(\frac{\overline{\lambda}}{\underline{\lambda}}\right)\right)$ instead of $\mathcal{O}\left(\frac{\overline{\lambda}}{\underline{\lambda}}\right)$ solves!

Transforming the integration region: results

(A, B) from structural engineering, $n = 1473$, seek 300 highest eigenpairs.

Order (p)	Transformation method		Gauß–Legendre		Trapezoidal rule	
4	300	eigenpairs	0	eigenpairs	65	eigenpairs
	9	iterations	10	iterations	10	iterations
	13k	solves	18k	solves	17k	solves
8	300	eigenpairs	0	eigenpairs	68	eigenpairs
	5	iterations	10	iterations	10	iterations
	14k	solves	36k	solves	35k	solves
16	300	eigenpairs	294	eigenpairs	82	eigenpairs
	2	iterations	**10**	iterations	**10**	iterations
	14k	solves	58k	solves	69k	solves

!

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