Polynomial and rational filtering for eigenvalue problems and the EVSL project

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Large eigenvalue problems in applications

➤ Challenge in eigenvalue problems: extract large number of eigenvalues & vectors of very large matrices (quantum physics/ chemistry, ...) - often in the middle of spectrum.

➤ Example: *Excited states* involve transitions $\longrightarrow$ much more complex computations than for DFT (ground states)

➤ Large matrices, *many* eigen-pairs to compute

Illustration:

'Hamiltonian of size $n \sim 10^6$ get 10% of bands'

Solving large interior eigenvalue problems

Three broad approaches:

1. Shift-invert (real shifts)
2. Polynomial filtering
3. Rational filtering (Cauchy, + others).

Issues with shift-and invert (and related approaches)

➤ Issue 1: factorization may be too expensive

- Can use iterative methods?

➤ Issue 2: Iterative techniques often fail –

- Reason: Highly indefinite problems.

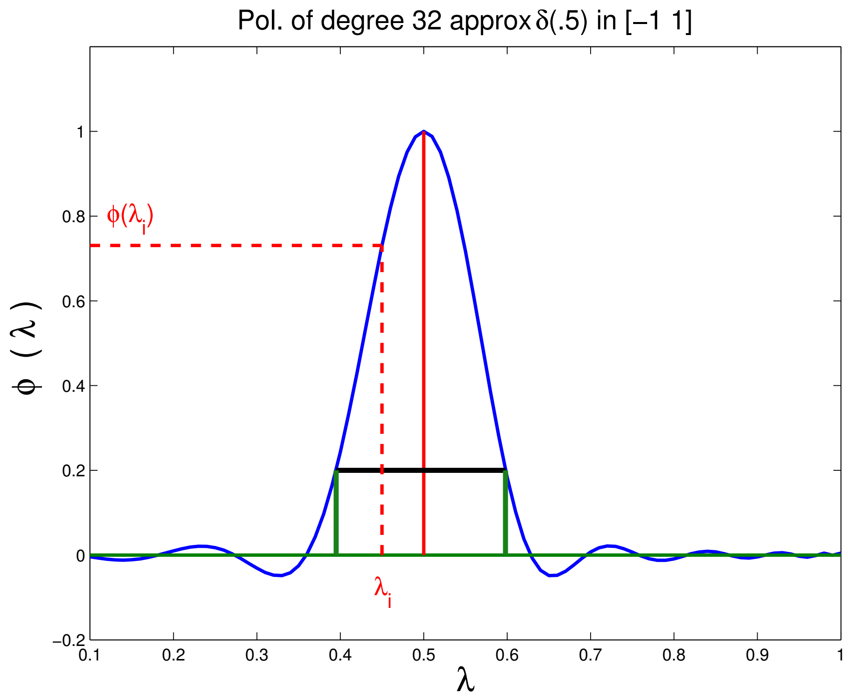
➤ First Alternative: ‘Spectrum slicing’ with Polynomial filtering

"Spectrum Slicing"

- Situation: very large number of eigenvalues to be computed
- Goal: compute spectrum by slices by applying filtering
- Apply Lanczos or Subspace iteration to problem:

$$\phi(A)u = \mu u$$

$\phi(t) \equiv$ a polynomial or rational function that enhances wanted eigenvalues



Rationale. Eigenvectors on both ends of wanted spectrum need not be orthogonalized against each other :

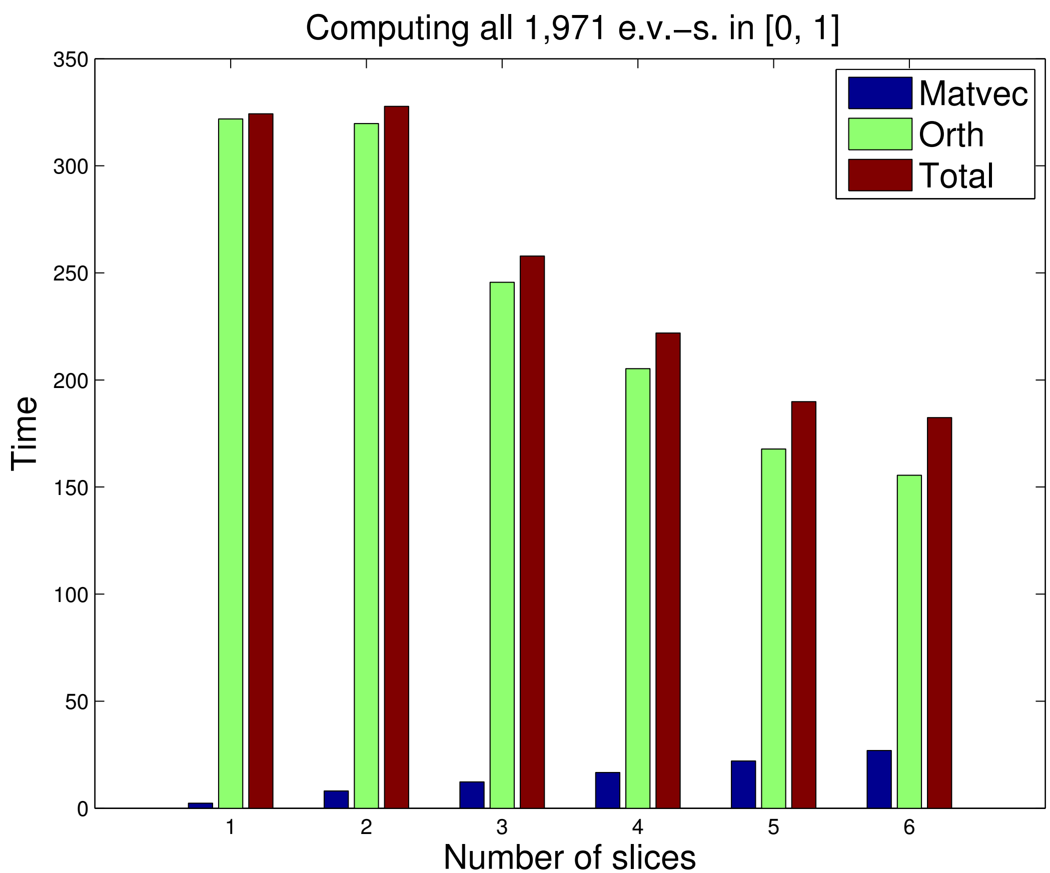
➤ Idea: Get the spectrum by ‘slices’ or ’windows’ [e.g., a few hundreds or thousands of pairs at a time]

➤ Can use polynomial or rational filters

*Hypothetical scenario: large A, *many* wanted eigenpairs*

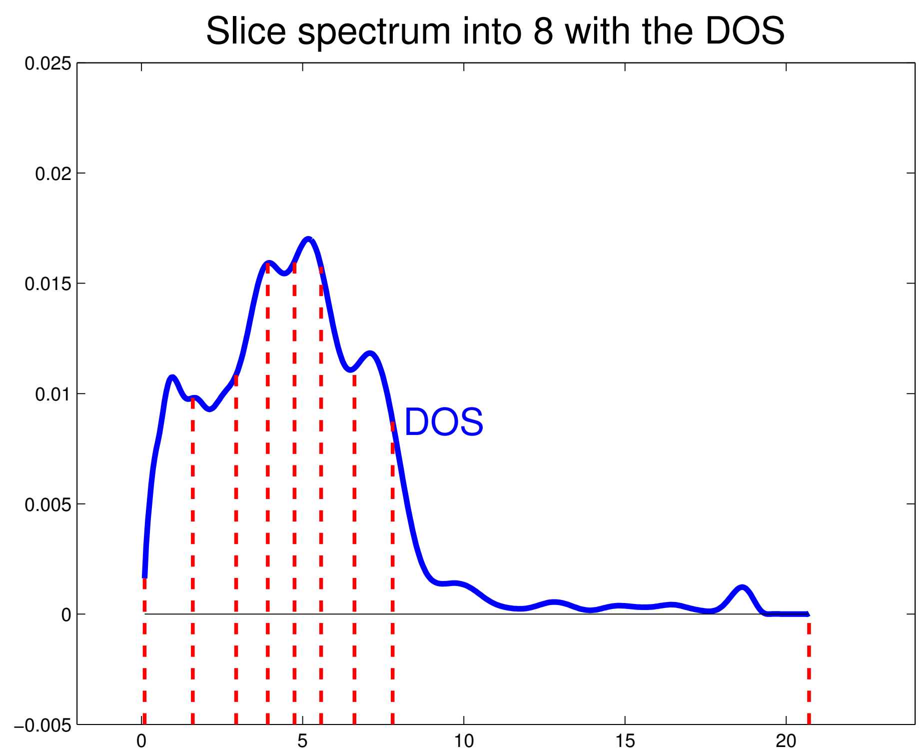
- Assume A has size $10M$
- ... and you want to compute 50,000 eigenvalues/vectors (huge for numerical analysits, not for physicists) ...
- ... in the lower part of the spectrum - or the middle.
- By (any) standard method you will need to orthogonalize at least 50K vectors of size 10M. Then:
  - Space needed: $\approx 4 \times 10^{12}$ b = 4TB *just for the basis*
  - Orthogonalization cost: 5×10^{16} = 50 PetaOPS.
  - At step k, each orthogonalization step costs $\approx 4kn$
  - This is $\approx 200,000n$ for k close to $50,000$.

Illustration: All eigenvalues in [0, 1] of a 49^3 Laplacean



Note: This is a small pb. in a scalar environment. Effect likely much more pronounced in a fully parallel case.

How do I slice my spectrum?



Answer: Use the DOS.

➤ We must have:

$$\int_{t_i}^{t_{i+1}} \phi(t)dt = \frac{1}{n_{slices}} \int_a^b \phi(t)dt$$

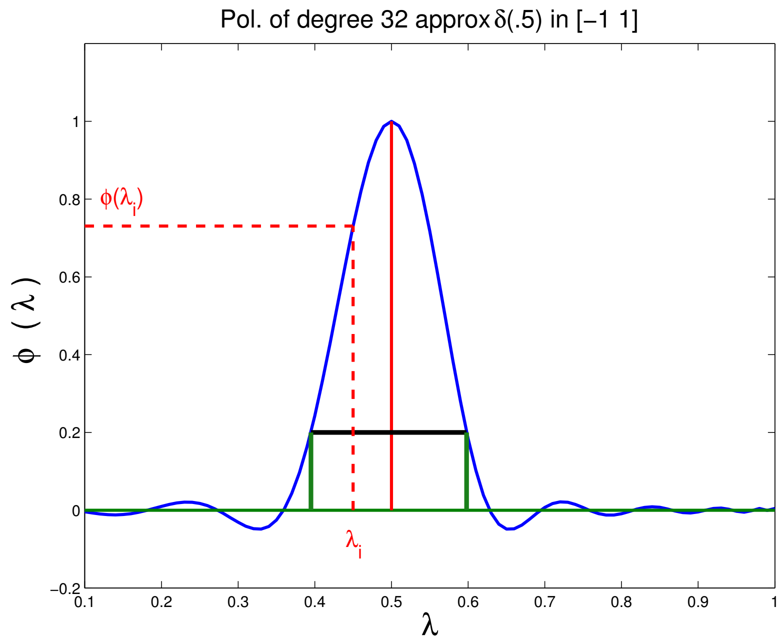
Polynomial filtering

- Apply Lanczos or Subspace iteration to: $\boxed{M = \rho(A)}$ where $\rho(t)$ is a polynomial
- Each *matvec* $y = Av$ is replaced by $y = \rho(A)v$.
- Eigenvalues in high part of filter will be computed first.
- Old (forgotten) idea. But new context is *very* favorable

What polynomials?

➤ LS approximations to δ-Dirac functions

➤ Obtain the LS approximation to the δ— Dirac function – Centered at some point (TBD) inside the interval. $\longrightarrow$



➤ W'll express everything in the interval $[-1, 1]$

Theory

The Chebyshev expansion of δ_γ is

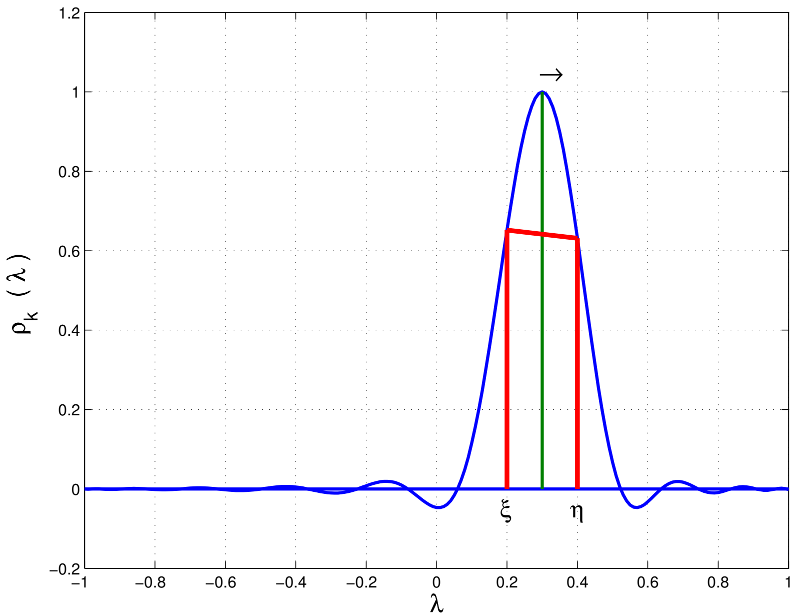
$$\rho_k(t) = \sum_{j=0}^{k} \mu_j T_j(t) \ \text{ with } \ \mu_j = \begin{cases} \frac{1}{2} & j = 0 \\ \cos(j \cos^{-1}(\gamma)) & j > 0 \end{cases}$$

➤ Recall: The delta Dirac function is not a function – we can't properly approximate it in least-squares sense. However:

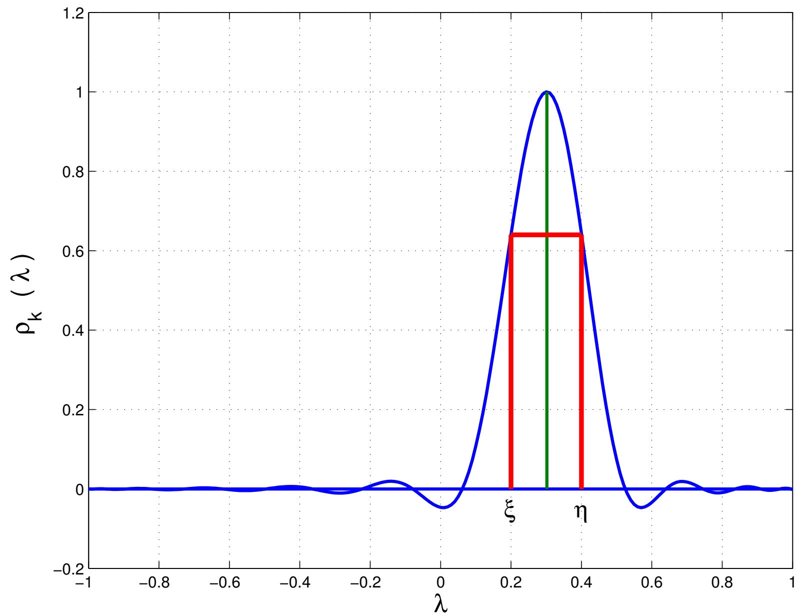
Proposition Let $\hat{\rho}_k(t)$ be the polynomial that minimizes $\|r(t)\|_w$ over all polynomials r of degree $\le k$, such that $r(\gamma) = 1$, where $\|.\|_w$ represents the Chebyshev L^2-norm. Then $\hat{\rho}_k(t) = \rho_k(t)/\rho_k(\gamma)$.

A few technical details. Issue # one: 'balance the filter'

- To facilitate the selection of *'wanted'* eigenvalues [Select λ's such that $\rho(\lambda) >$ bar] we need to ...
- ... find γ so that $\rho(\xi) == \rho(\eta)$



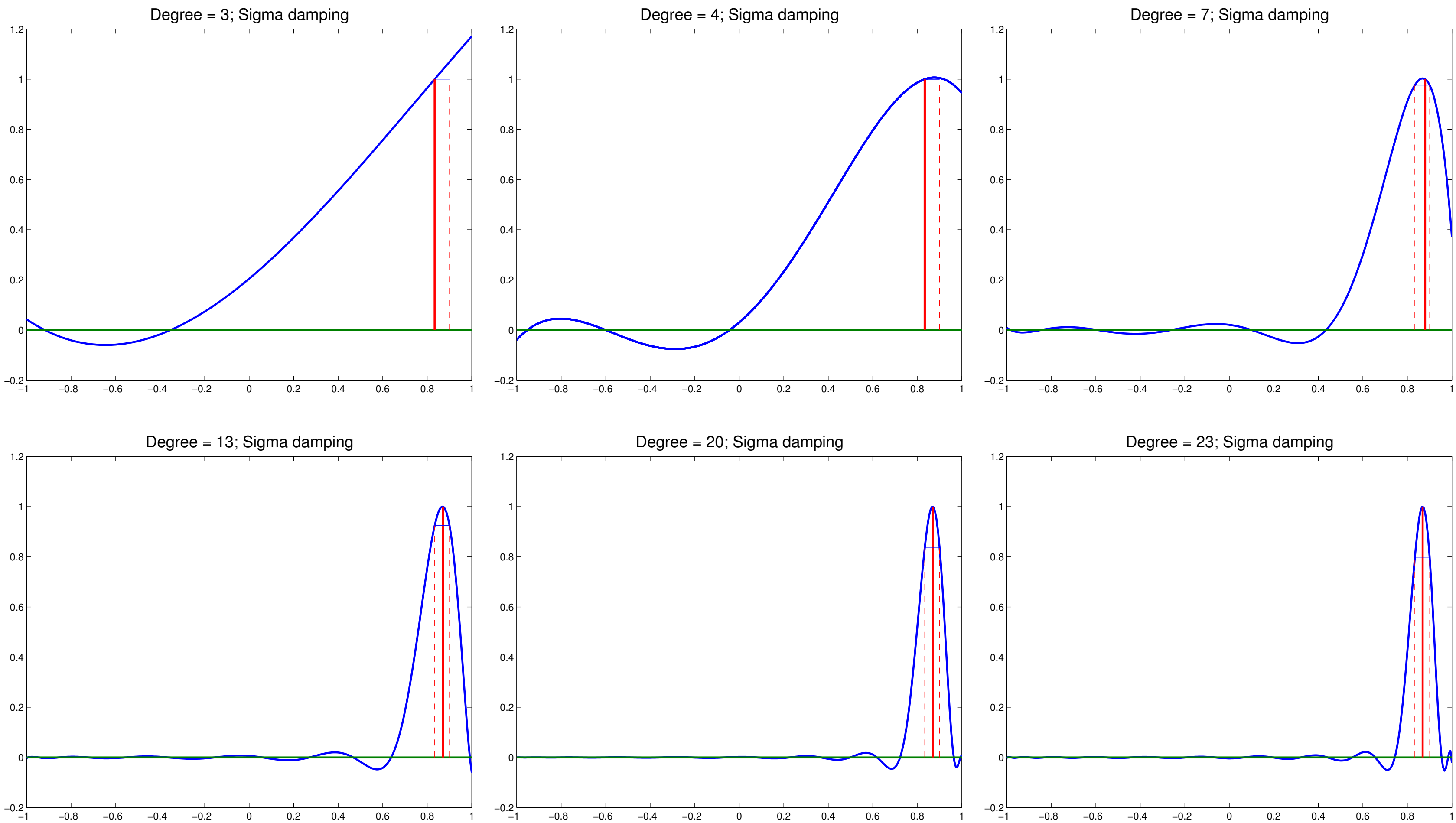
$\longrightarrow$



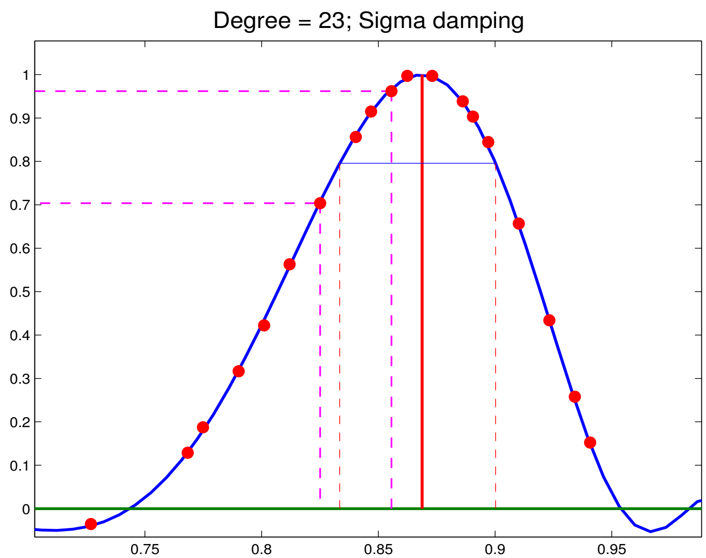
Procedure: Solve the equation $\rho_\gamma(\xi) - \rho_\gamma(\eta) = 0$ with respect to γ, accurately. Use Newton or eigenvalue formulation.

Issue # two: Determine degree & polynomial (automatically)

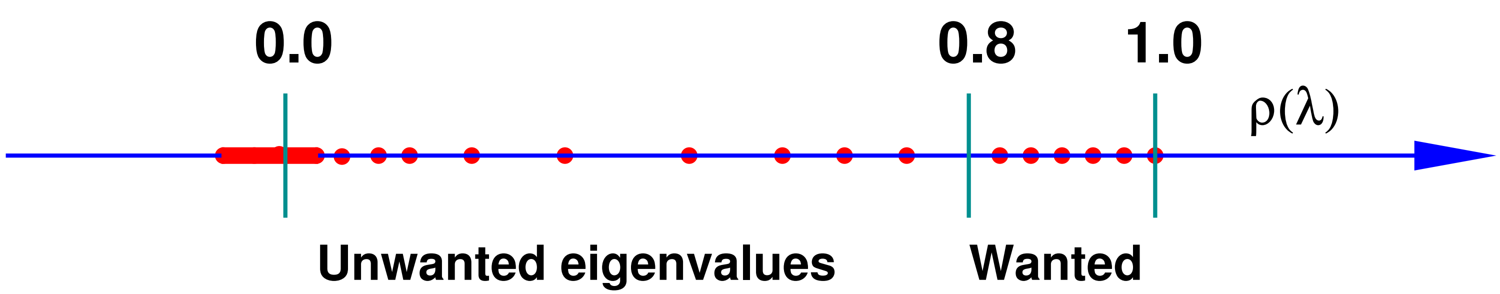
Start low then increase degree until value (s) at the boundary (ies) become small enough - Exple for [0.833, 0.907..]



Polynomial filtered Lanczos: No-Restart version

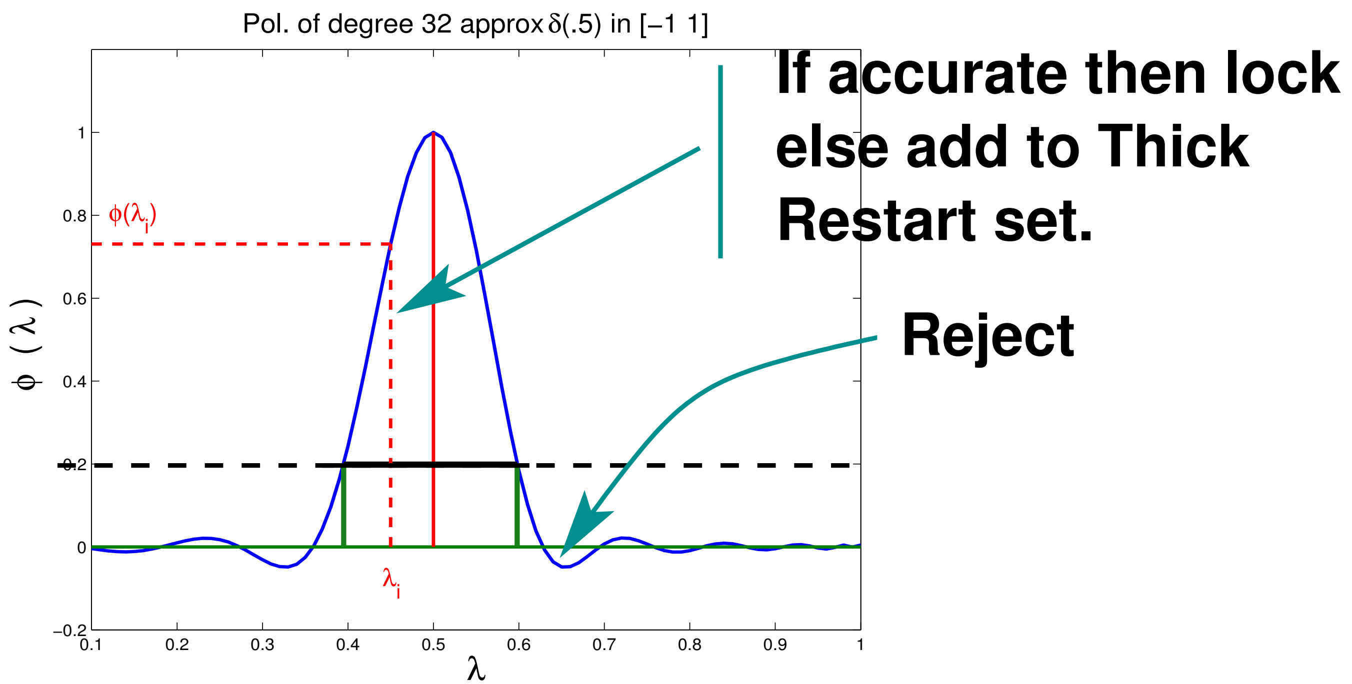


- Use Lanczos with full reorthogonalization on $\rho(A)$. Eigenvalues of $\rho(A)$: $\rho(\lambda_i)$
- Accept if $\rho(\lambda_i) \geq$ `bar`
- Ignore if $\rho(\lambda_i) <$ `bar`



Polynomial filtered Lanczos: Thick-Restart version

➤ PolFilt Thick-Restart Lanczos in a picture:

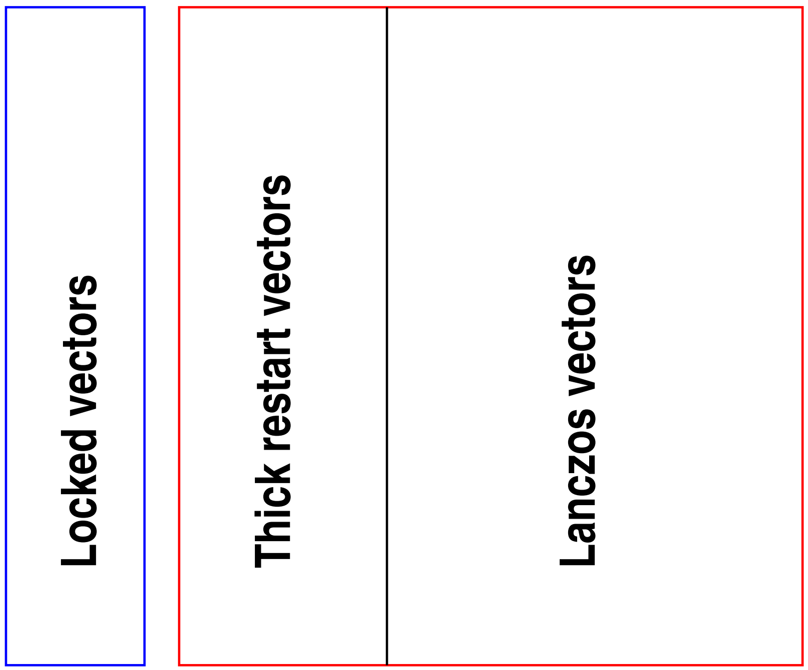


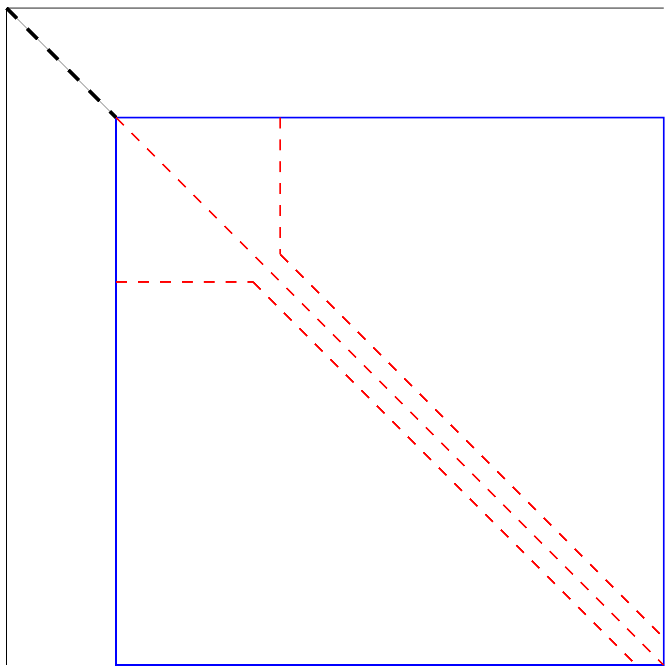
➤ Due to locking, no more candidates will show up in wanted area after some point $\rightarrow$ Stop.

TR Lanczos: The 3 types of basis vectors

Basis vectors

Matrix representation





Experiments: Hamiltonian matrices from PARSEC

Matrix	n	$\sim$ nnz	$[a, b]$	$[\xi, \eta]$	$\nu_{[\xi,\eta]}$
$\mathbf{Ge_{87}H_{76}}$	$\mathbf{112,985}$	$\mathbf{7.9}M$	$[-\mathbf{1.21, 32.76}]$	$[-\mathbf{0.64}, -\mathbf{0.0053}]$	212
$\mathbf{Ge_{99}H_{100}}$	$\mathbf{112,985}$	$\mathbf{8.5}M$	$[-\mathbf{1.22, 32.70}]$	$[-\mathbf{0.65}, -\mathbf{0.0096}]$	250
$\mathbf{Si_{41}Ge_{41}H_{72}}$	$\mathbf{185,639}$	$\mathbf{15.0}M$	$[-\mathbf{1.12, 49.82}]$	$[-\mathbf{0.64}, -\mathbf{0.0028}]$	218
$\mathbf{Si_{87}H_{76}}$	$\mathbf{240,369}$	$\mathbf{10.6}M$	$[-\mathbf{1.19, 43.07}]$	$[-\mathbf{0.66}, -\mathbf{0.0300}]$	213
$\mathbf{Ga_{41}As_{41}H_{72}}$	$\mathbf{268,096}$	$\mathbf{18.5}M$	$[-\mathbf{1.25, 1301}]$	$[-\mathbf{0.64}, -\mathbf{0.0000}]$	201

Results: (No-Restart Lanczos)

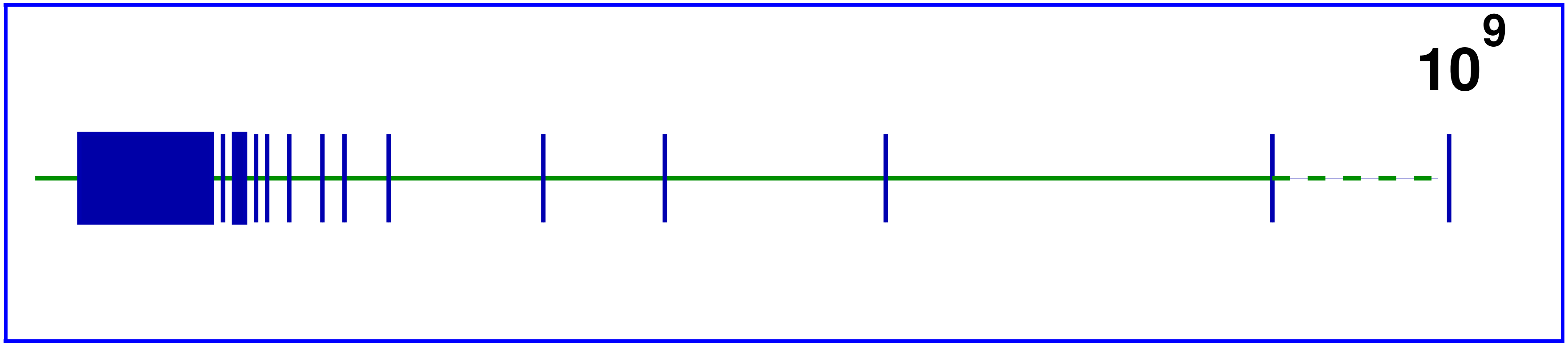
Matrix	deg	iter	matvec	CPU time (sec)			max residual
				matvec	orth.	total	
$Ge_{87}H_{76}$	26	1,020	26,784	48.58	18.67	74.45	1.20×10^{-12}
$Ge_{99}H_{100}$	26	1,090	28,642	60.11	20.44	86.52	7.20×10^{-12}
$Si_{41}Ge_{41}H_{72}$	32	950	30,682	105.05	28.25	144.19	1.20×10^{-10}
$Si_{87}H_{76}$	29	1,010	29,561	76.45	39.16	128.95	4.30×10^{-12}
$Ga_{41}As_{41}H_{72}$	174	910	158,889	693.5	34.16	759.99	3.70×10^{-12}

➤ Demo with Si10H16 [$n = 17,077, \ nnz(A) = 446,500$]

RATIONAL FILTERS

Why use rational filters?

- Consider a spectrum like this one:



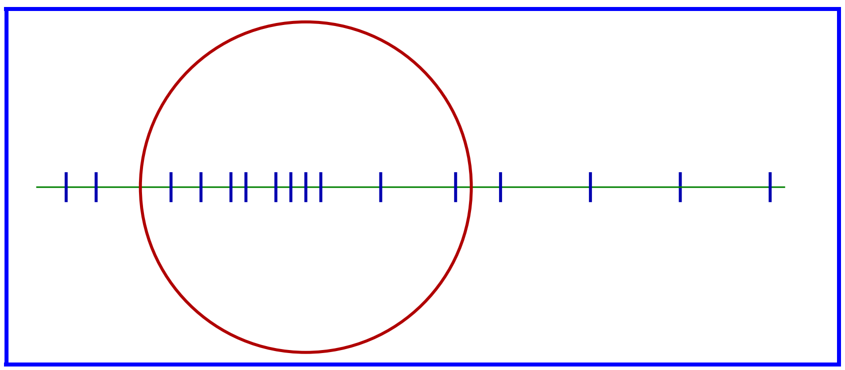
- Polynomial filtering utterly ineffective for this case
- Second issue: situation when Matrix-vector products are expensive
- Generalized eigenvalue problems.

- Alternative is to use rational filters:

$$\phi(z) = \sum_j \frac{\alpha_j}{z-\sigma_j}$$

$$\phi(A) = \sum_j \alpha_j (A - \sigma_j I)^{-1}$$ $\rightarrow$ We now need to solve linear systems

- Tool: Cauchy integral representations of spectral projectors

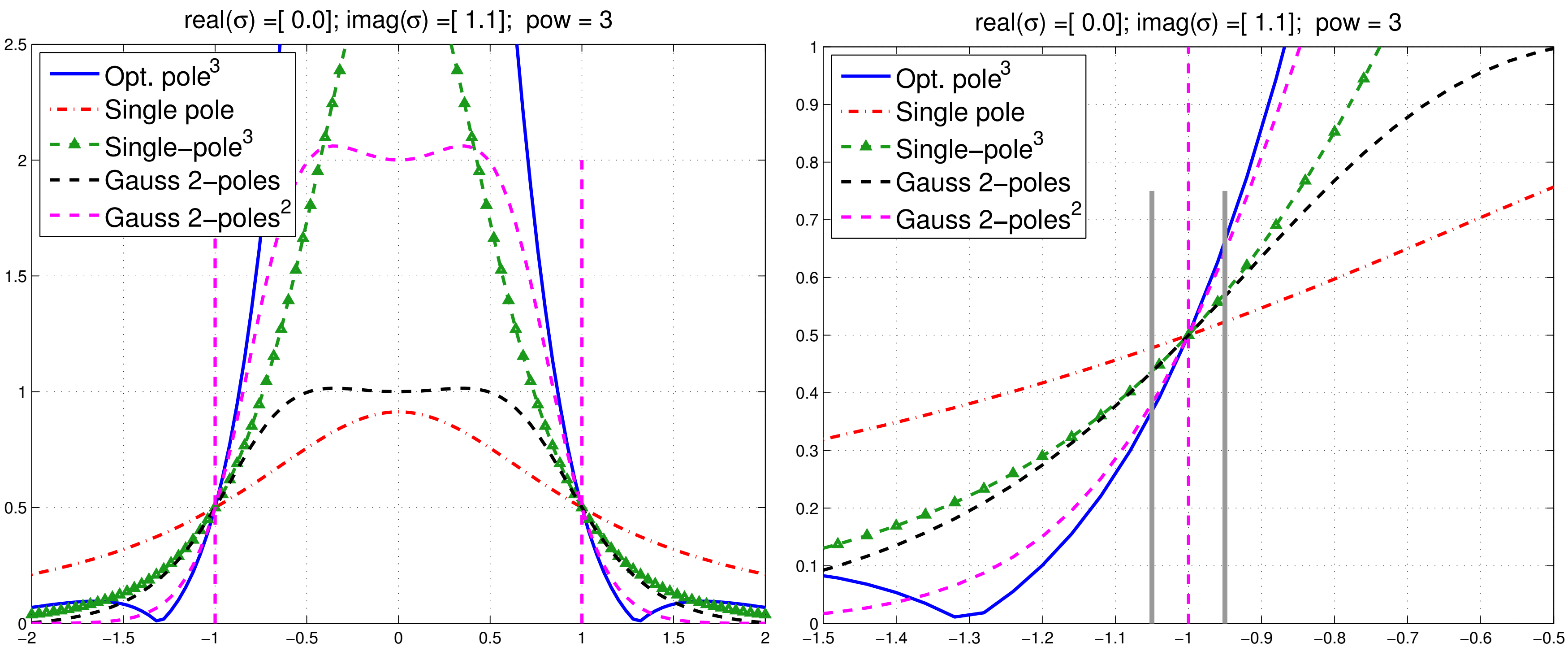


$$P = \frac{-1}{2i\pi} \int_\Gamma (A - sI)^{-1} ds$$

- Numer. integr. $P \rightarrow \tilde{P}$
- Use Krylov or S.I. on $\tilde{P}$

- Sakurai-Sugiura approach [Krylov]
- FEAST [Subs. iter.] (E. Polizzi)

What makes a good filter



- Assume subspace iteration is used with above filters. Which filter will give better convergence?

- Simplest and best indicator of performance of a filter is the magnitude of its derivative at -1 (or 1)

The Gauss viewpoint: Least-squares rational filters

- Given: poles $\sigma_1, \sigma_2, \cdots, \sigma_p$
- Related basis functions $\phi_j(z) = \frac{1}{z - \sigma_j}$

Find $\phi(z) = \sum_{j=1}^{p} \alpha_j \phi_j(z)$ that minimizes

$$\int_{-\infty}^{\infty} w(t)|h(t) - \phi(t)|^2 dt$$

- $h(t)$ = step function $\chi_{[-1,1]}$.
- $w(t)$= weight function.

For example $a = 10$,
$\beta = 0.1$

$$w(t) = \begin{cases} 0 \text{ if } & |t| > a \\ \beta \text{ if } & |t| \le 1 \\ 1 \text{ else} & \end{cases}$$

➤ Advantages:

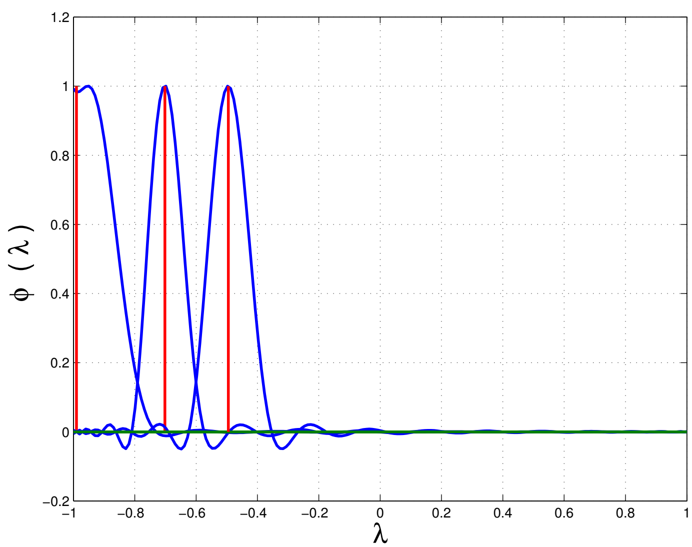
- Can select poles far away from real axis $\rightarrow$ faster iterative solvers
- Very flexible – can be adapted to many situations
- Can repeat poles (!)

➤ Implemented in EVSL.. [Interfaced to `SuiteSparse` as a solver]

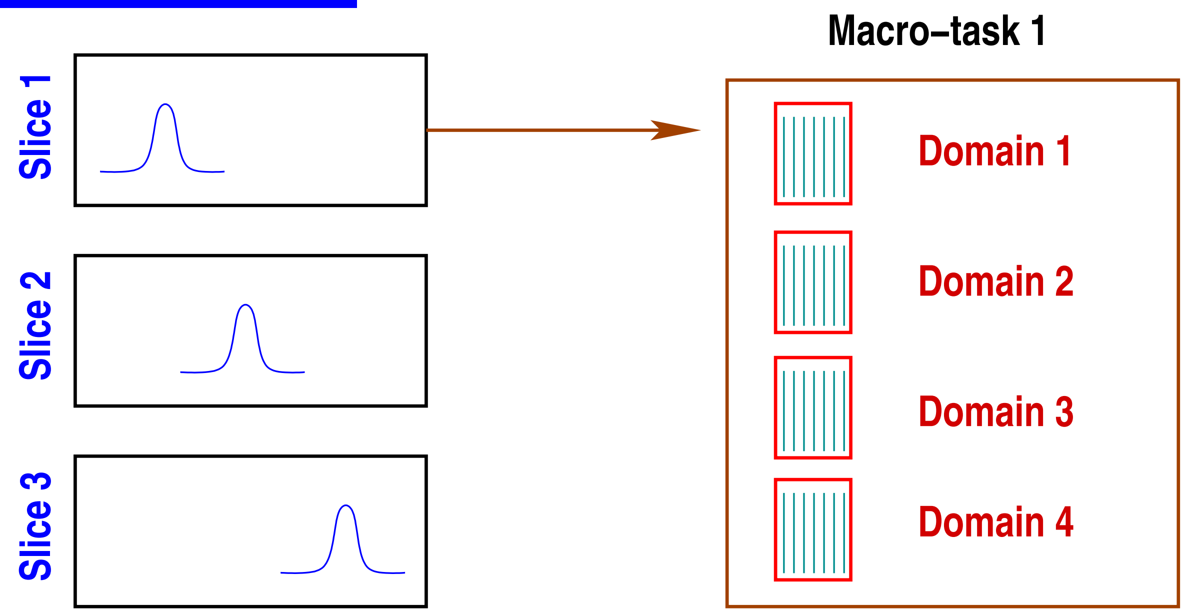
Spectrum Slicing and the EVSL project

- Newly released EVSL uses polynomial and rational filters
- Each can be appealing in different situations.

Spectrum slicing: cut the overall interval containing the spectrum into small sub-intervals and compute eigenpairs in each sub-interval independently.



Levels of parallelism



The two main levels of parallelism in EVSL

EVSL web-page - Mozilla Firefox

Yousef Saad -- SOFTWARE × EVSL web-page ×

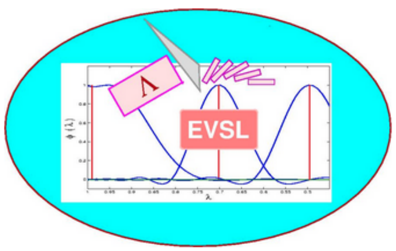
www-users.cs.umn.edu/~saad/software/EVSL/index.html 90% Ruipeng Li

Most Visited UoM Mail Home - Dropbox Research.gov - User L... Gmail OneStop : Welcome t... Google Accounts Live Statistics | Revolv... Setting up a repositor...

E V S L : *EigenValues Slicing Library* -- (Version 1.0)

This version dated : Thu Jan 26 15:24:02 CST 2017
New version to be posted (~ July 2017)

E . V . S . L .



Welcome to the first release of EVSL (the EigenValues Slicing Library). EVSL provides routines for computing eigenvalues located in a given interval, and their associated eigenvectors, of a real symmetric matrix. It also provides tools for spectrum slicing, i.e., the technique of subdividing a given interval into p smaller subintervals and computing the eigenvalues in each subinterval independently. EVSL implements a polynomial filtered Lanczos (thick restart, no restart) a rational filtered Lanczos (thick restart, no restart), and a polynomial filtered subspace iteration.
The technical reports listed below provide details on the techniques used in the package. **Online documentation** (based on Doxygen) is now available - see below.
The package will see frequent updates. We are currently working on various **interfaces to Fortran**.
Note: A new version of EVSL - with much added functionality - will be released in the next few weeks (Some time at the end of May/early June'17).

http://www.cs.umn.edu/~saad/software

Related publications

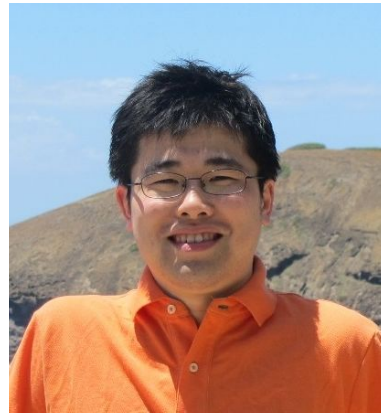
- **Ruipeng Li, Yuanzhe Xi, Eugene Vecharynski, Chao Yang, and Yousef Saad.**
  A Thick-Restart Lanczos algorithm with polynomial filtering for Hermitian eigenvalue problems. SIAM J. Sci. Comput., 38 (2016), pp. A2512-A2534. Preprint ys-2015-6, Dept. Computer Science and Engineering **Download: [PDF]**

Download EVSL

Before you download read the COPYRIGHT statement

Download: EVSL version 1.0 (EVSL_1.0.zip)

EVSL Main Contributors (version 1.1.0) + support



- Ruipeng Li
LLNL

- Yuanzhe Xi
Post-doc (UMN)

- Luke Erlandson
UG Intern (UMN)

➤ Work supported by DOE [ending this summer] ...

... and by NSF [going forward]

EVSL: current status & plans

Version _1.0 Released in Sept. 2016

- Matrices in CSR format (only)
- Standard Hermitian problems (no generalized)
- Spectrum slicing with KPM (Kernel Polynomial Meth.)
- Trivial parallelism across slices with OpenMP
- Methods:
  - Non-restart Lanczos – polynomial & rational filters
  - Thick-Restart Lanczos – polynomial & rational filters
  - Subspace iteration – polynomial & rational filters

Version _1.1.x V_1.1.0 Due for release end of July

- general `matvec` [passed as function pointer]
- $Ax = \lambda Bx$
- Fortran (03) interface.
- Spectrum slicing by Lanczos and KPM
- Efficient Spectrum slicing for $Ax = \lambda Bx$ (no solves with B).

Version _1.2.x V_1.2.0 Early 2018 (?)

- Fully parallel version [MPI + openMP]
- Challenge application in earth sciences [in progress]

Conclusion

- Polynomial Filtering appealing when # of eigenpairs to be computed is large and Matvecs are not too expensive
- Somewhat costly for generalized eigenvalue problems
- Will not work well for spectra with large outliers.
- Alternative: Rational filtering –
- Both approaches implemented in EVSL
- Current focus: provide as many interfaces as possible.
- `EVSL` code available here:

  `www.cs.umn.edu/~saad/software/EVSL`

- `EVSL` Also on github (development)