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Filtering techniques for eigenvalue problems

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Background. Origins of Eigenvalue Problems

- Structural Engineering [$\boldsymbol{Ku = \lambda Mu}$] (Goal: frequency response)
- Electronic structure calculations [Schrödinger equation..]
- Stability analysis [e.g., electrical networks, mechanical system,..]
- Bifurcation analysis [e.g., in fluid flow]

➤ Large eigenvalue problems in quantum chemistry use up biggest portion of the time in supercomputer centers

Background. New applications in data analytics

➤ Machine learning problems often require a (partial) *Singular Value Decomposition* -

➤ Somewhat different issues in this case:

- Very large matrices, update the SVD
- Compute dominant singular values/vectors
- Many problems of approximating a matrix (or a tensor) by one of lower rank (Dimension reduction, ...)

➤ But: Methods for computing SVD often based on those for standard eigenvalue problems

Background. The Problem (s)

- Standard eigenvalue problem:

$$\boldsymbol{Ax = \lambda x}$$

Often: $\boldsymbol{A}$ is symmetric real (or Hermitian complex)

- Generalized problem $\boldsymbol{Ax = \lambda Bx}$ Often: $\boldsymbol{B}$ is symmetric positive definite, $\boldsymbol{A}$ is symmetric or nonsymmetric

- Quadratic problems: $\boldsymbol{(A + \lambda B + \lambda^2 C)u = 0}$

- Nonlinear eigenvalue problems (NEVP)

$$\boxed{\left[\boldsymbol{A_0 + \lambda B_0 + \sum_{i=1}^{n} f_i(\lambda) A_i}\right] \boldsymbol{u = 0}}$$

- General form of NEVP $\boxed{A(\lambda)x = 0}$
- Nonlinear eigenvector problems:

$$[A + \lambda B + F(u_1, u_2, \cdots, u_k)]u = 0$$

What to compute:

- A few λ_i 's with smallest or largest real parts;
- All λ_i's in a certain region of $\mathbb{C}$;
- A few of the dominant eigenvalues;
- All λ_i's (rare).

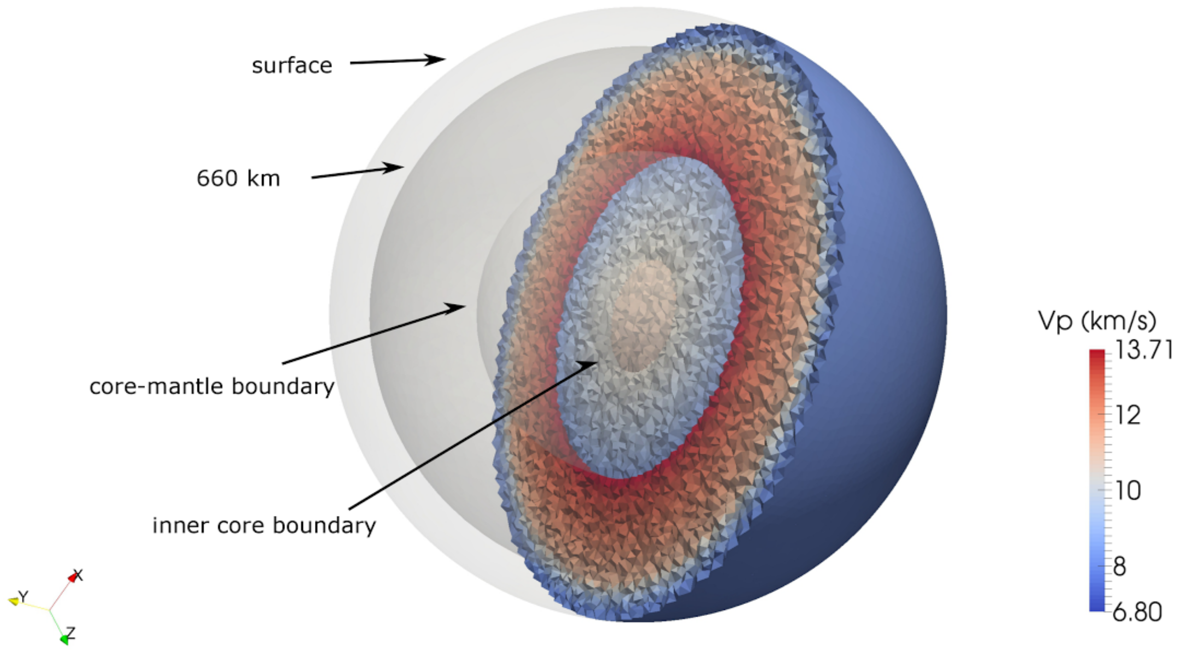
Large eigenvalue problems in applications

➤ Some applications require the computation of a large number of eigenvalues and vectors of very large matrices.

➤ Density Functional Theory in electronic structure calculations: *'ground states'*

➤ *Excited states* involve transitions and invariably lead to much more complex computations. $\longrightarrow$ Large matrices, *many* eigen-pairs to compute

Computing earth normal modes (J. Shi & M. V. De Hoop)



- FEM model leads to a generalized eigenvalue problem
- Compute (a large number of) eigenvalues in an interval
- More on this later

Background: The main tools

Projection process:

(a) Build a 'good' subspace $K = \mathbf{span}(V)$;

(b) get approximate eigenpairs by a Rayleigh-Ritz process:
$\tilde{\lambda}$, $\tilde{u} \in K$ satisfy: $(A - \tilde{\lambda} I)\tilde{u} \perp K \longrightarrow$

$$\boxed{V^H(A - \tilde{\lambda} I)Vy = 0}$$

- ➤ $\tilde{\lambda}$ = Ritz value, $\tilde{u} = Vy$ = Ritz vector
- ➤ Two common choices for K:
  1) Power subspace $K = \mathbf{span}\{A^k X_0\}$; or $\mathbf{span}\{P_k(A)X_0\}$;
  2) Krylov subspace $K = \mathbf{span}\{v, Av, \cdots, A^{k-1}v\}$

Background. The main tools (cont)

Shift-and-invert:

- If we want eigenvalues near σ, replace A by $(A - \sigma I)^{-1}$.

Example: power method: $v_j = Av_{j-1}/$scaling replaced by

$$\boxed{v_j = \frac{(A-\sigma I)^{-1} v_{j-1}}{\text{scaling}}}$$

- Works well for computing *a few* eigenvalues near σ/
- Used in commercial package NASTRAN (for decades!)
- Requires factoring $(A - \sigma I)$ (or $(A - \sigma B)$ in generalized case.) But convergence will be much faster.
- A solve each time - Factorization done once (ideally).

Background. The main tools (cont)

Deflation:

➤ Once eigenvectors converge remove them from the picture

Restarting Strategies :

➤ Restart projection process by using information gathered in previous steps

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➤ ALL available methods use some combination of these ingredients.

[e.g. ARPACK: Arnoldi/Lanczos + ‘implicit restarts’ + shift-and-invert (option).]

Solving large eigenvalue problems: Current state-of-the art

- Eigenvalues at one end of the spectrum:
  - Subspace iteration + filtering [e.g. FEAST, Cheb,...]
  - Lanczos+variants (no restart, thick restart, implicit restart, Davidson,..), e.g., ARPACK code, PRIMME.
  - Block Algorithms [Block Lanczos, TraceMin, LOBPCG, SlepSc,...]
  - + Many others - more or less related to above
- 'Interior' eigenvalue problems (middle of spectrum):
  - Combine shift-and-invert + Lanczos/block Lanczos. Used in, e.g., NASTRAN
  - Rational filtering [FEAST, Sakurai et al.,..]

Solving large interior eigenvalue problems

Three broad approaches:

1. Shift-invert: $A \longrightarrow (A - \sigma I)^{-1}$
2. Polynomial filtering: $A \longrightarrow p(A)$
3. Rational filtering: $A \rightarrow \sum \alpha_i (A - \sigma_i I)^{-1}$

Issues with shift-and invert (and related approaches)

➤ Direct methods for the solves may be too expensive

- Why not use iterative methods?

➤ Iterative techniques often fail –

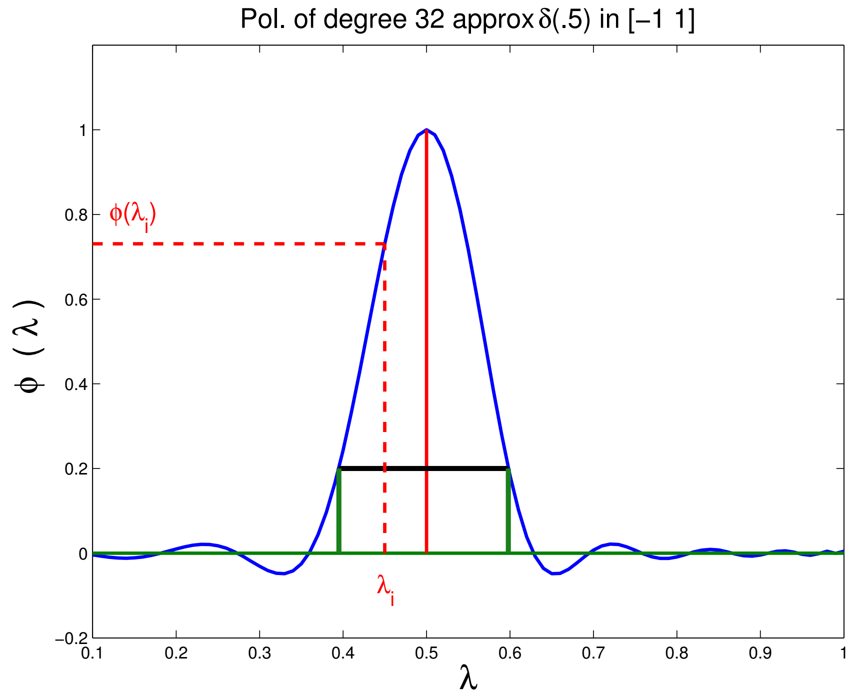
- Reason: Highly indefinite problems.

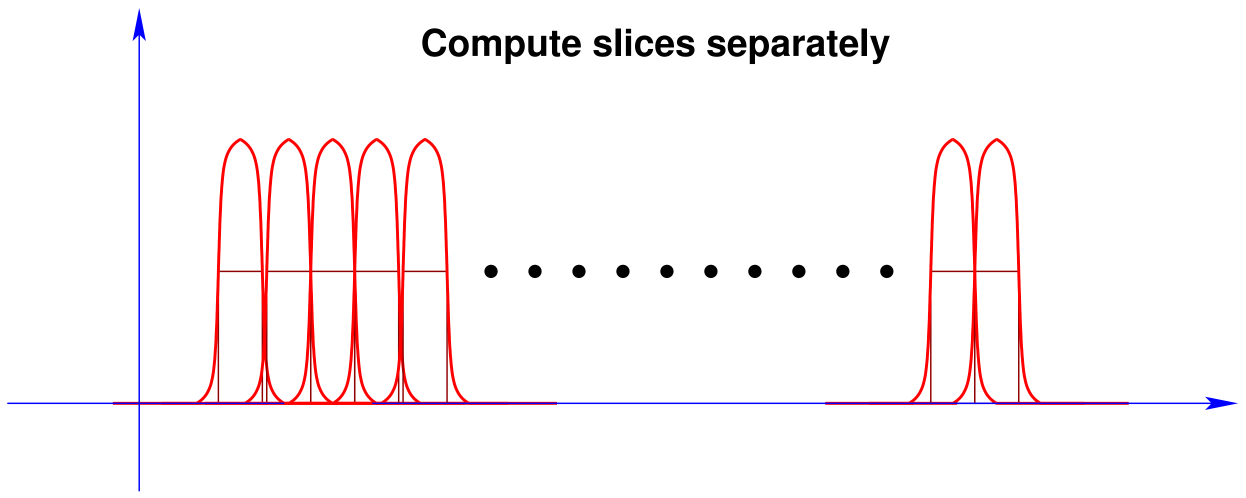
Filtering and "Spectrum Slicing"

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

$$\boxed{\phi(A)u = \mu u}$$

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

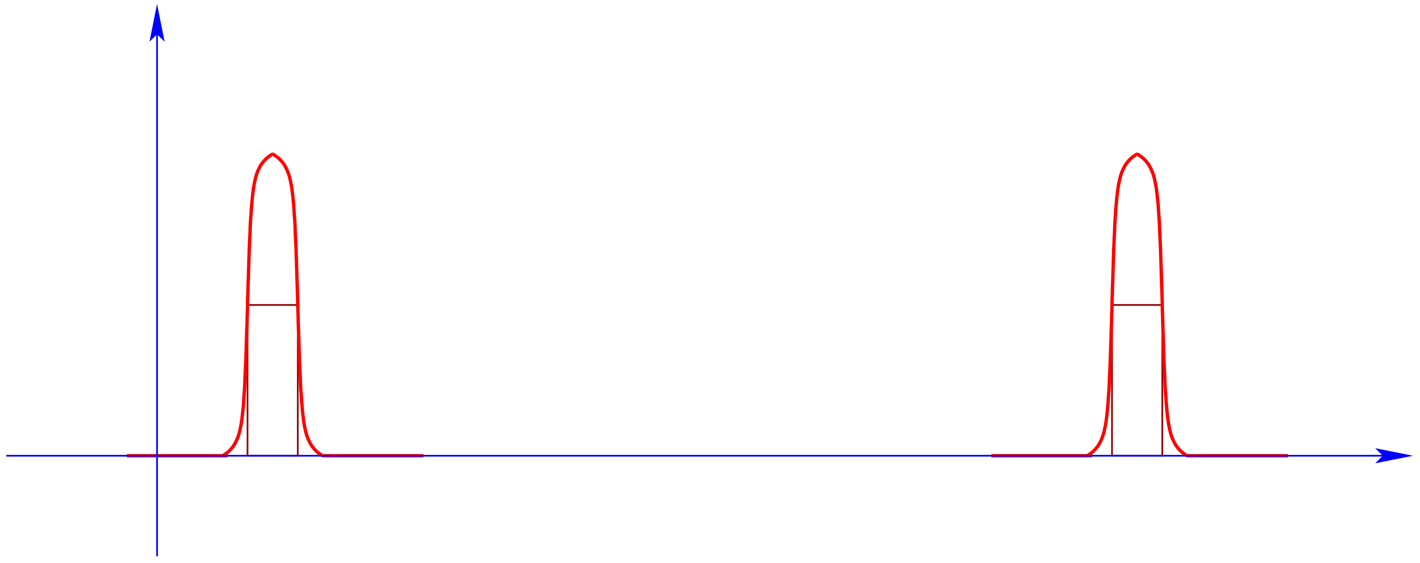




-
```
For each slice Do:
    [get *all* eigenpairs in a slice]
EndDo
```

Goal: Compute each slice independently from the others.

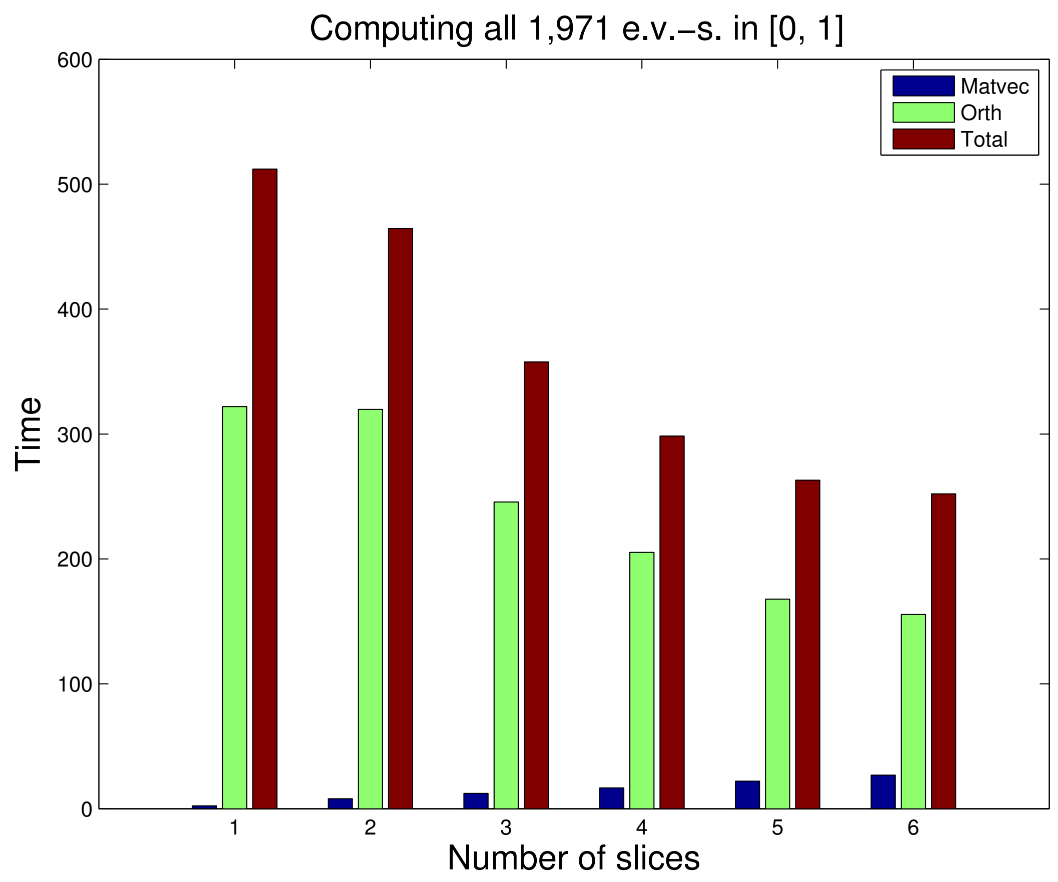
Rationale. Eigenvectors associated with different slices need not be orthogonalized against each other :



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

➤ Note: Orthogonalization + RR cost can be very high if we do not slice the spectrum

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.

POLYNOMIAL FILTERS

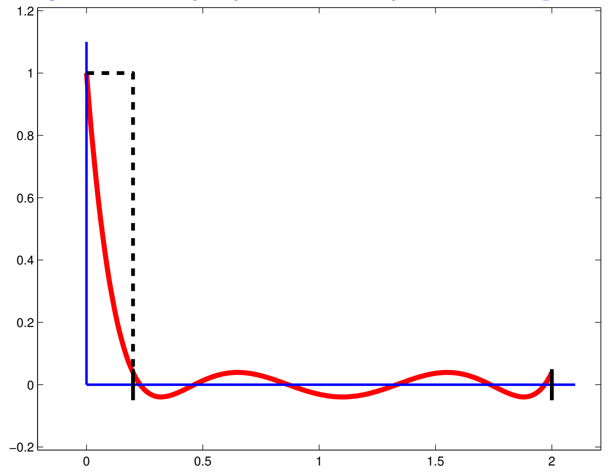
Polynomial filtering

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

What polynomials?

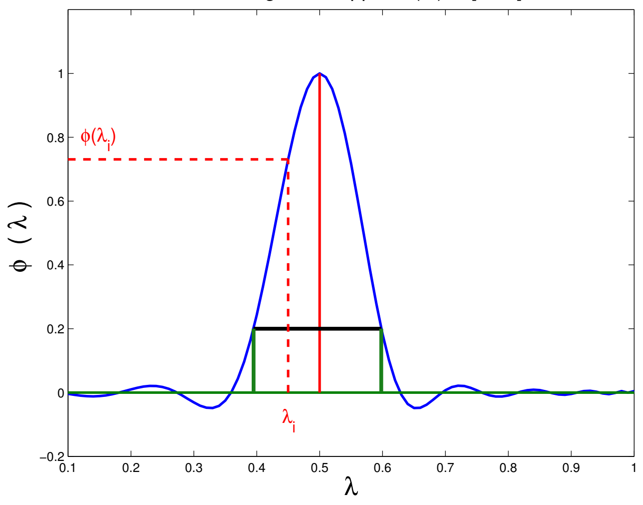
➤ For end-intervals: use standard Chebyshev polynomials (1st kind)

Deg. 6 Cheb. polynom., damped interv=[0.2, 2]



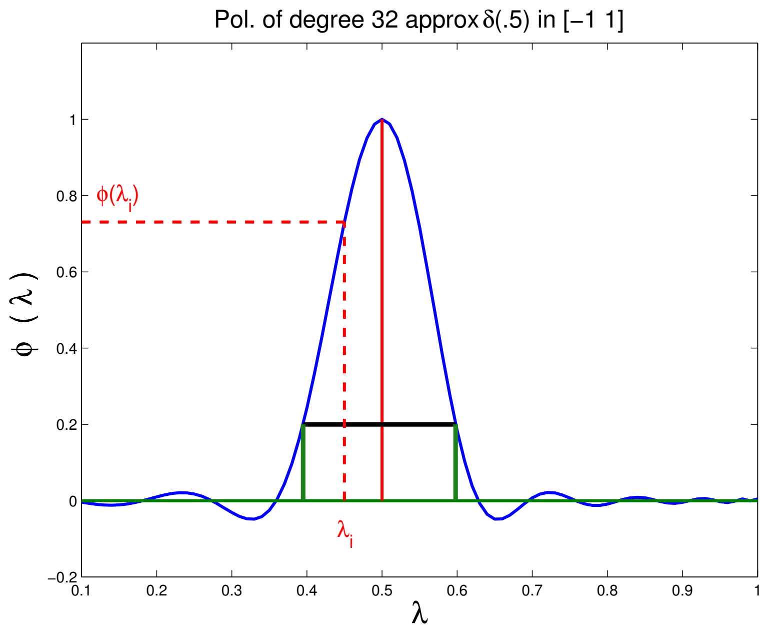
➤ For 'interior case' we need *a polynomial that has large values for* $\boldsymbol{\lambda} \in [\boldsymbol{a}, \boldsymbol{b}]$ *small values elsewhere*

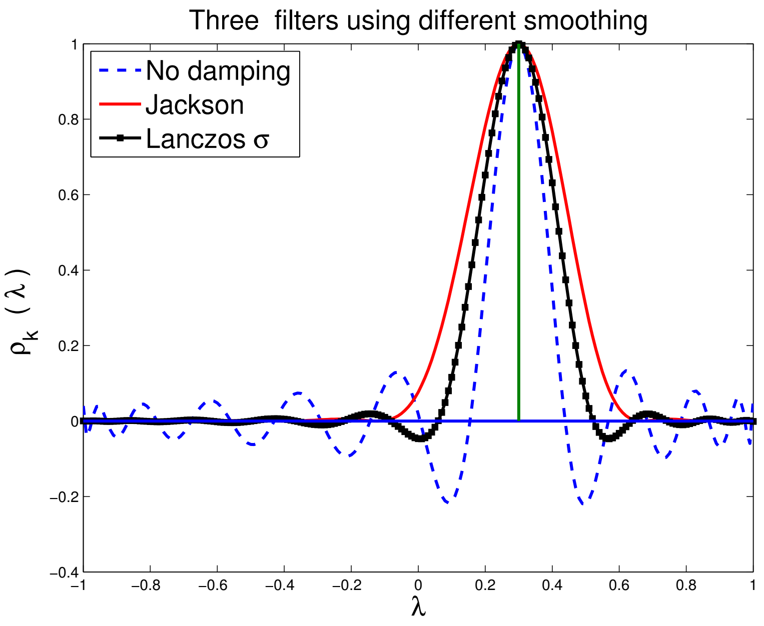
Pol. of degree 32 approx δ(.5) in [−1 1]



Simplest technique: δ-Dirac function

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





$\longleftarrow$ Can use same damping: Jackson, Lanczos σ damping, or none.

Theory

The Chebyshev expansion of δ_γ is

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

➤ 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 $\leq k$, such that $r(\gamma) = 1$, where $\|.\|_w$ represents the Chebyshev L^2-norm. Then $\hat{\rho}_k(t) = \rho_k(t)/\rho_k(\gamma)$.

‘The soul of a new filter’ – A few technical details

$$p_m(t) = \sum_{j=0}^{m} \gamma_j^{(m)} \mu_j T_j(t)$$

$$\mu_k = \begin{cases} 1/2 & \text{if } k == 0 \\ \cos(k \cos^{-1}(\gamma)) & \text{otherwise} \end{cases}$$

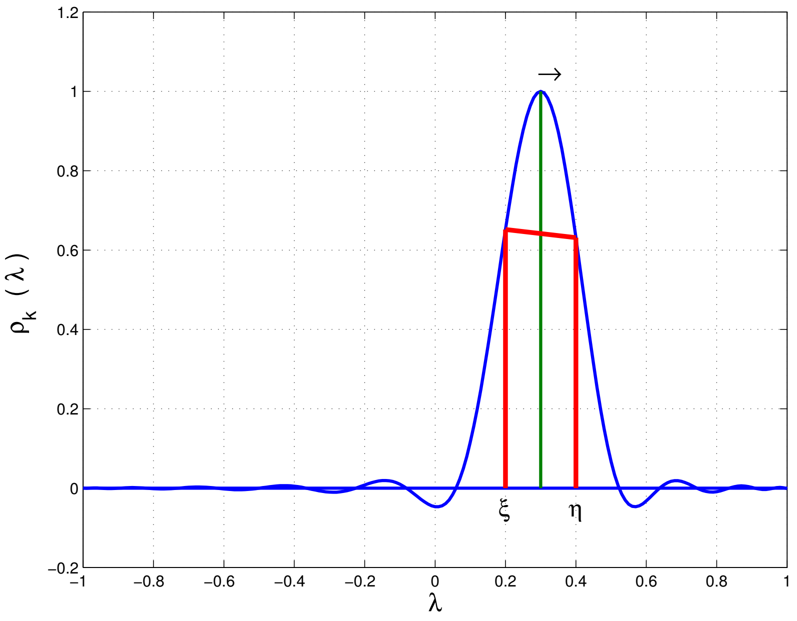
$$\gamma_j^{(m)} = \text{Damping coefficients.}$$

- quite simple...
- .. provided we handle a few practical issues

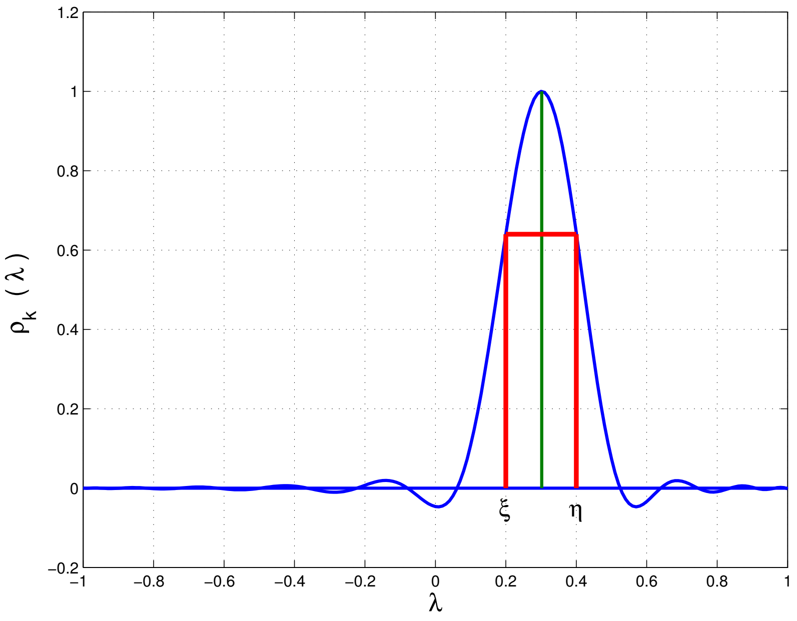
Issue # one: 'balance the filter'

➤ To facilitate the selection of *'wanted'* eigenvalues [Select $\boldsymbol{\lambda}$'s such that $\phi(\boldsymbol{\lambda}) >$ bar] we need to ...

➤ ... find γ so that $\phi(\boldsymbol{\xi}) == \phi(\boldsymbol{\eta})$

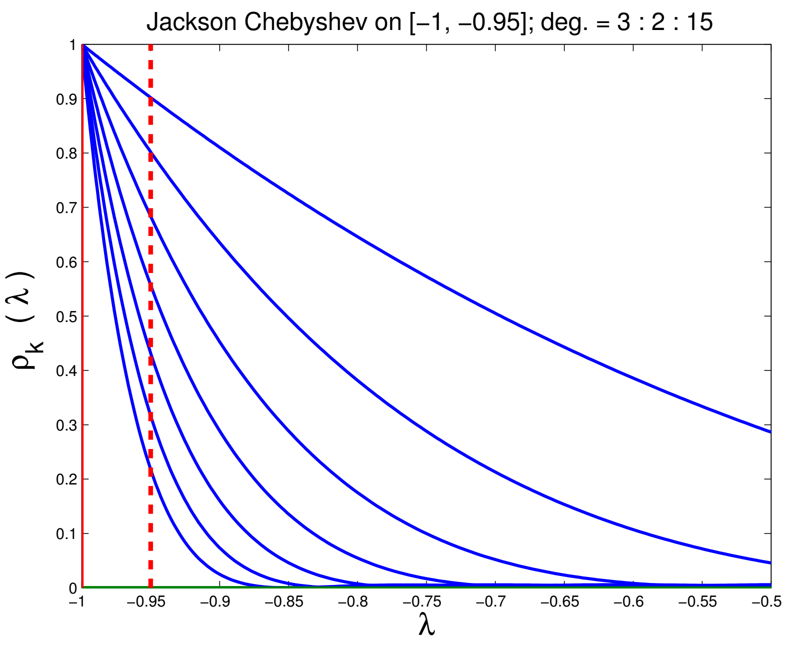


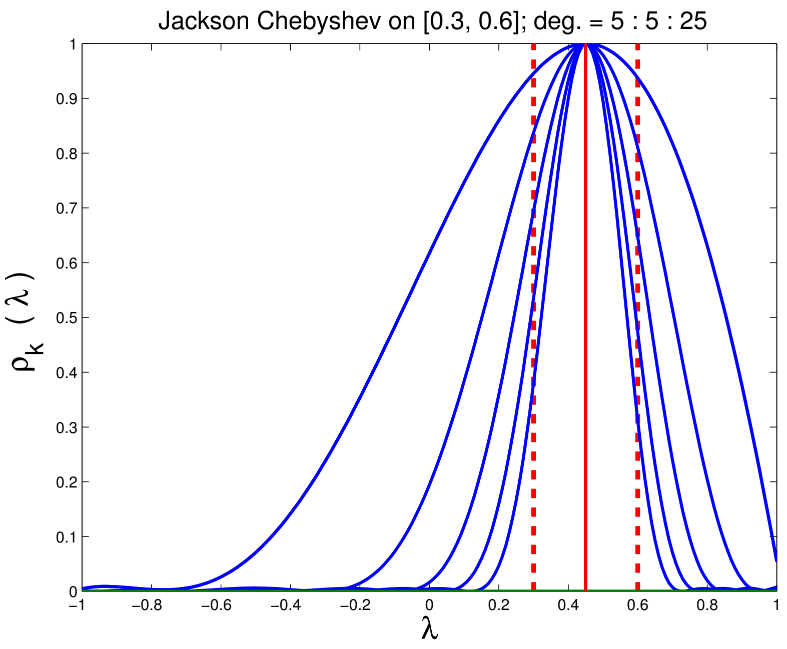
$\longrightarrow$



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

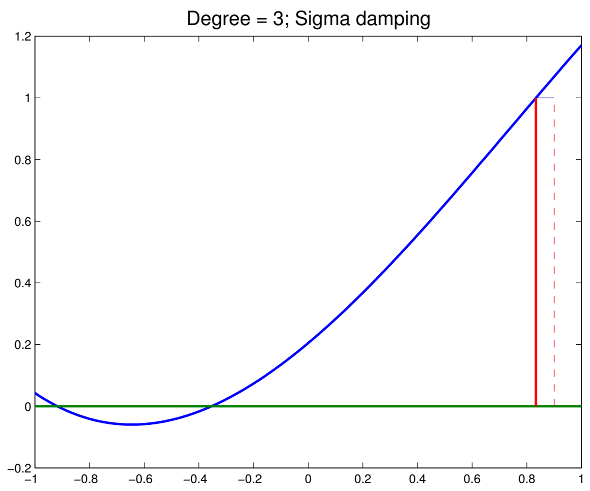
Issue # two: Determine degree & polynomial (automatically)

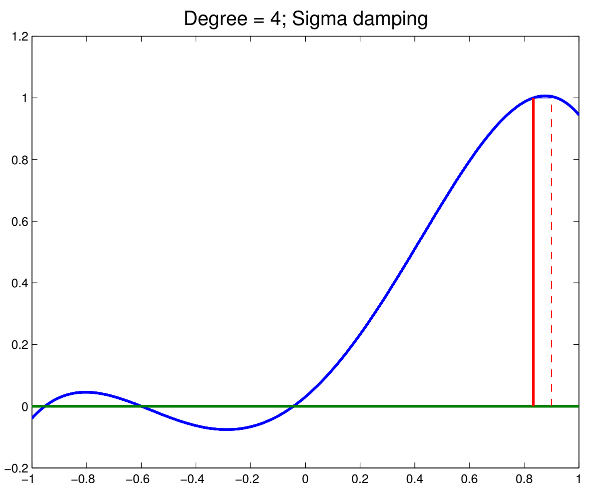


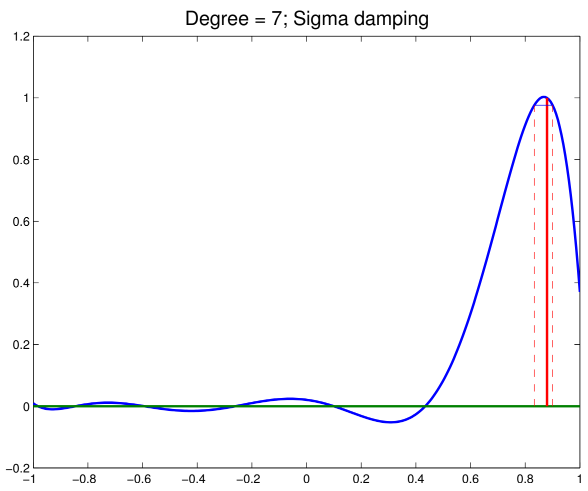


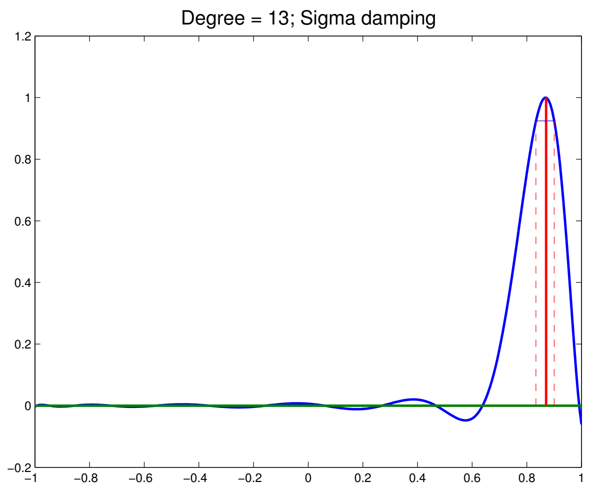
➤ 1) Start low (e.g. 2); 2) Increase degree until value (s) at the boundary (ies) become small enough –

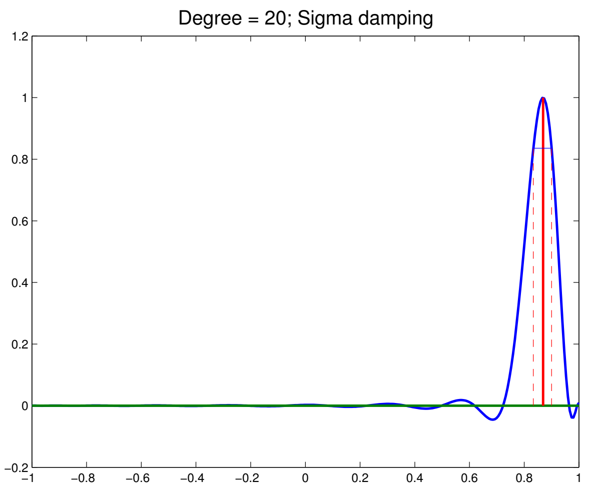
➤ Can also use criterion based on derivatives at ξ & η

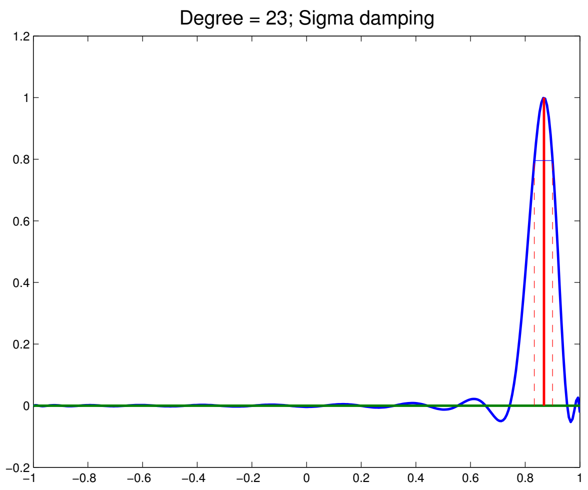

Degree = 3; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1

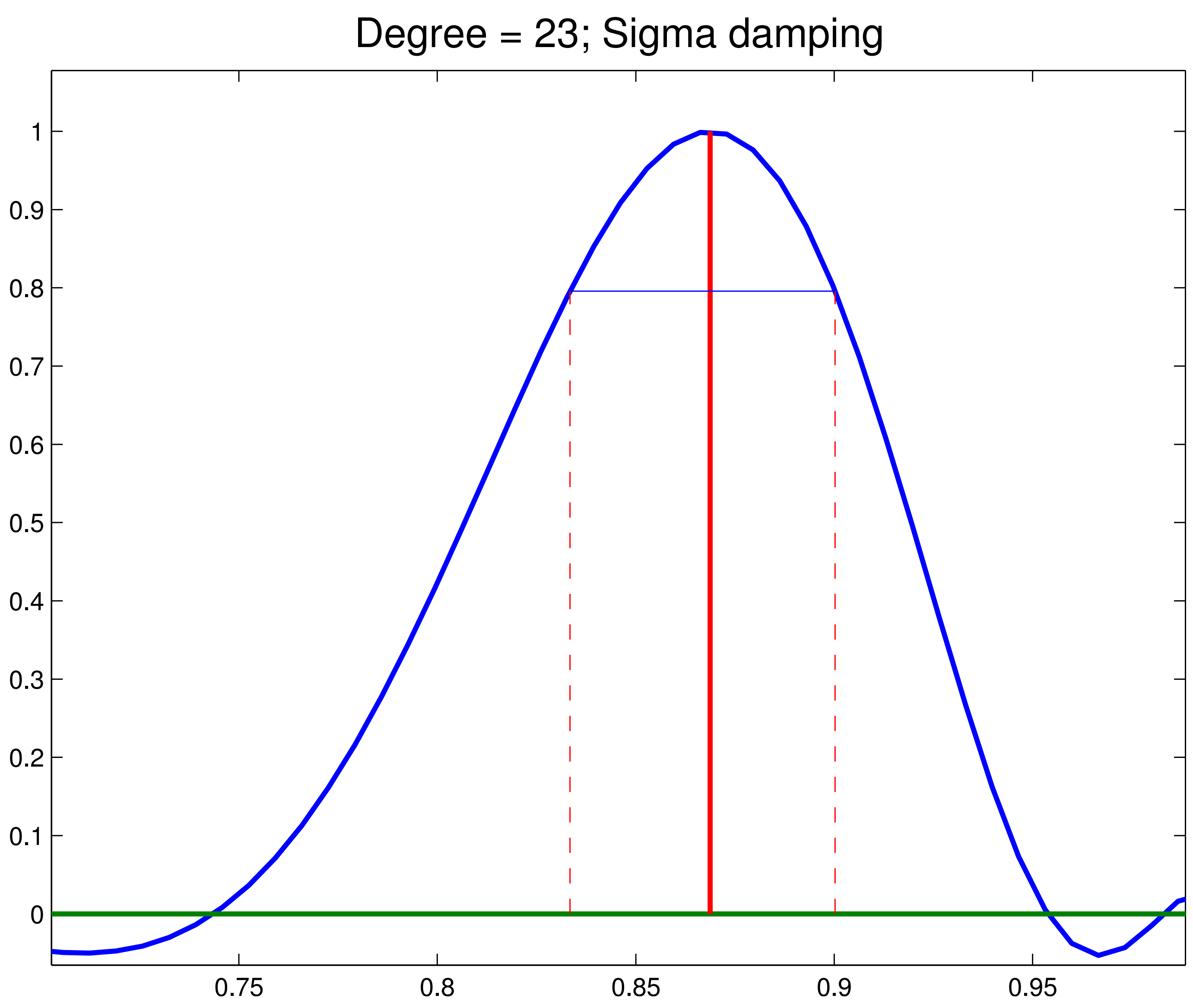

Degree = 4; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1


Degree = 7; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1


Degree = 13; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1


Degree = 20; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1

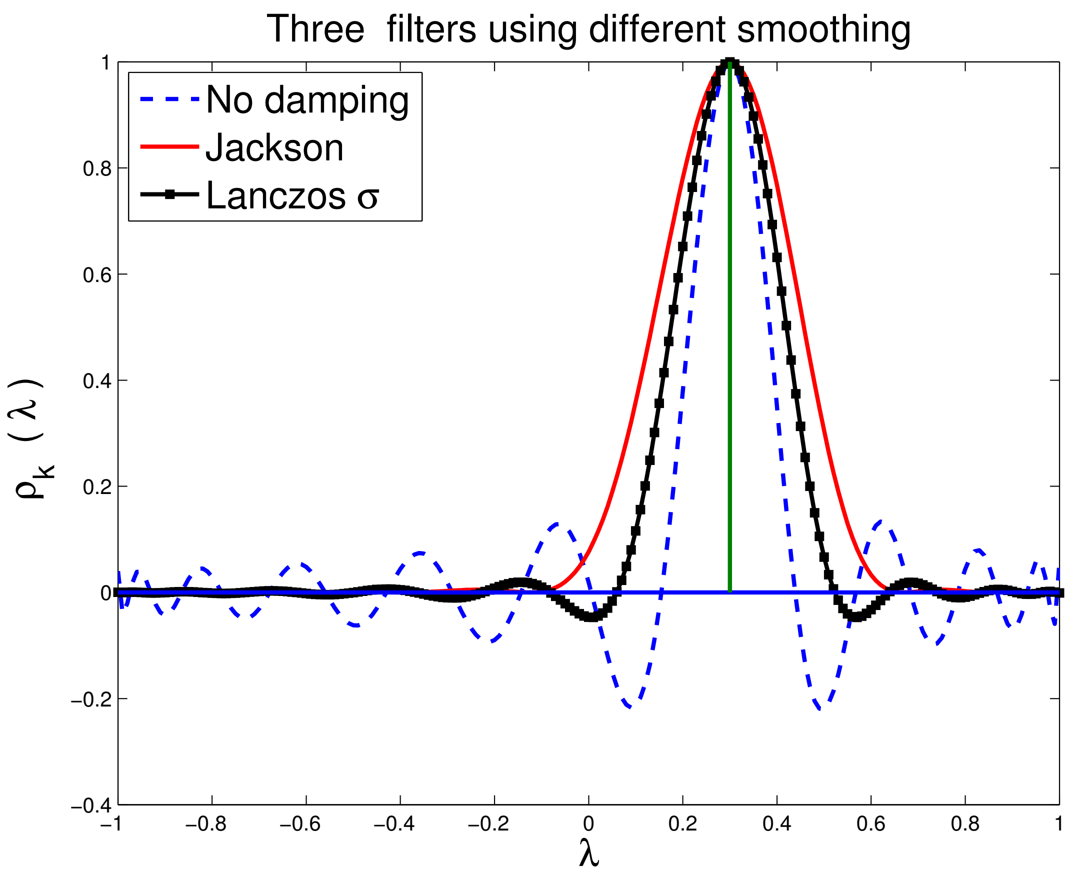

Degree = 23; Sigma damping
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1



A zoom on the final polynomial found

Issue # Three : Gibbs oscillations

- Discontinuous ‘function’ approximated $\to$ Gibbs oscillations



- Three options:

  - No damping
  - Jackson damping
  - Lanczos σ damping

- Good compromise: Lanczos σ damping

COMBINING FILTERING WITH A PROJECTION METHOD

Backround: The Lanczos Algorithm

- Algorithm builds orthonormal basis $V_m = [v_1, v_2, \cdots, v_m]$ for the Krylov subspace: $\text{span}\{v_1, Av_1, \cdots, A^{m-1}v_1\}$

- ... such that: $V_m^H A V_m = T_m$ - with

$$T_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & . & . & . & \\ & & & . & . & . \\ & & & & \beta_m & \alpha_m \end{pmatrix}$$

- Note: three term recurrence:

$$\boxed{\beta_{j+1}v_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}}$$

- Eigenvalues of A on both ends of spectrum are well approximated by eigenvalues of T_m (Ritz values).

Which Projection: Lanczos,w/o restarts, Subspace iteration,..

Options:

➤ Subspace iteration: quite appealing in some applications (e.g., electronic structure): $\boxed{\text{Can re-use previous subspace.}}$

➤ Simplest: (+ most efficient) Lanczos without restarts

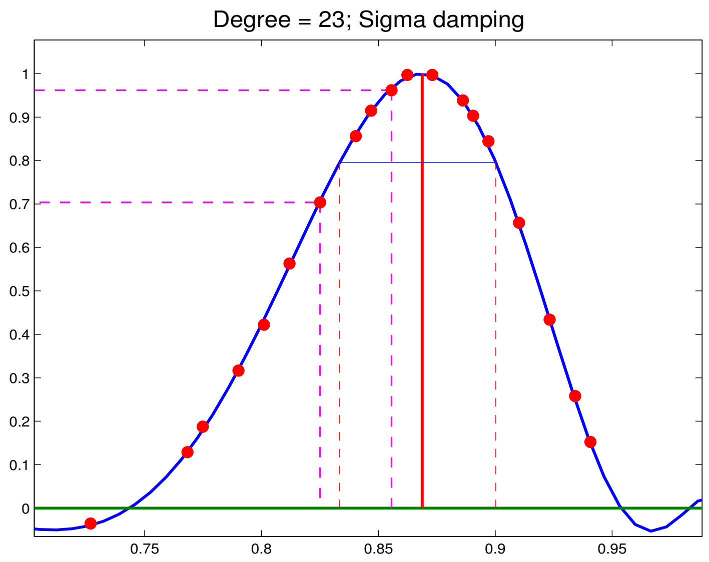
➤ Lanczos with Thick-Restarting [TR Lanczos, Stathopoulos et al '98, Wu & Simon'00]

➤ Crucial tool in TR Lanczos: deflation ('Locking')

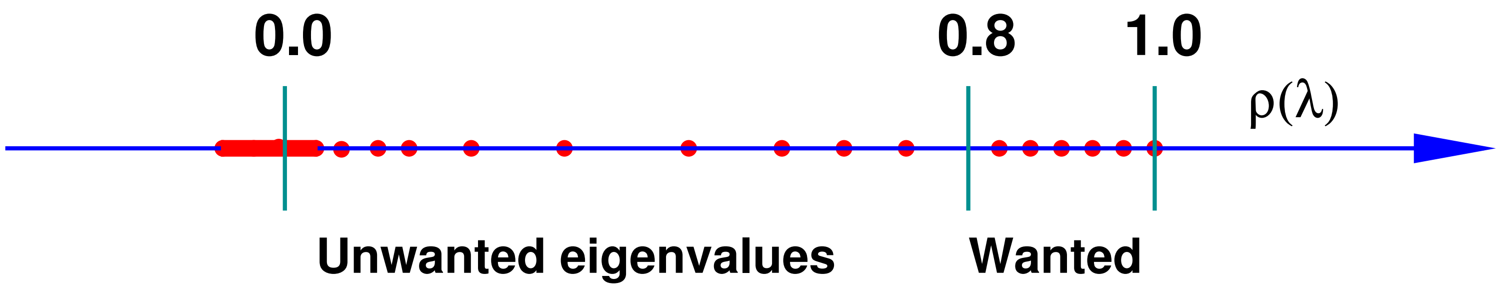
Main idea: *Keep extracting eigenvalues in interval* $[\xi, \eta]$ *until none are left.*

➤ If filter is good: Can catch all eigenvalues in interval

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`



How do I slice a spectrum?

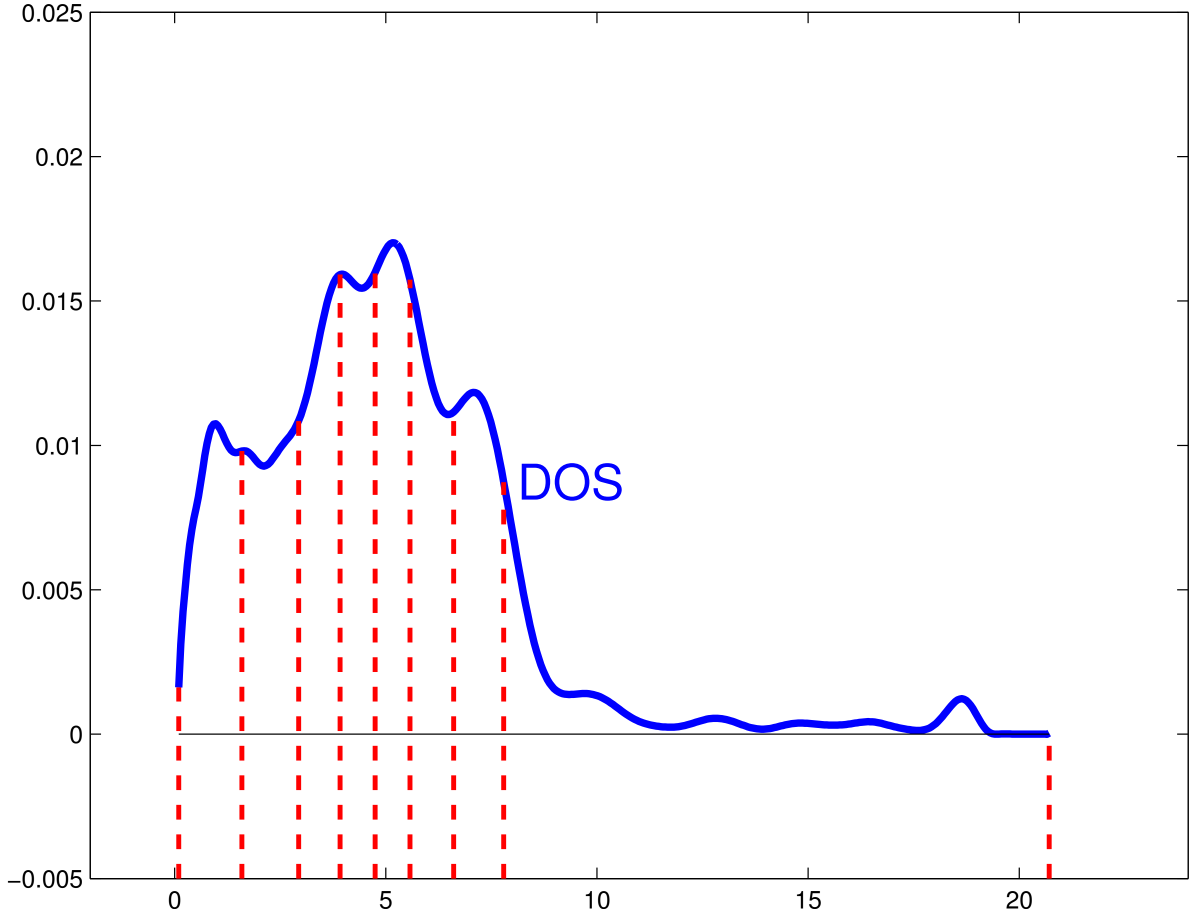
➤ Tools: Density of States (used in EVSL) or eigenvalue counts (used in FEAST)

- L. Lin, YS, Chao Yang [Siam review '16] – E. Di Napoli, E. Polizzi, YS ['16]
- KPM method – see, e.g., : *[Weisse, Wellein, Alvermann, Fehske, '06]*
- $\boxed{\text{Interesting instance of a tool from physics used in linear algebra.}}$

➤ Misconception: *'load balancing will be assured by just having slices with roughly equal numbers of eigenvalues'*

➤ In fact - will help mainly in balancing memory usage..

Slice spectrum into 8 with the DOS



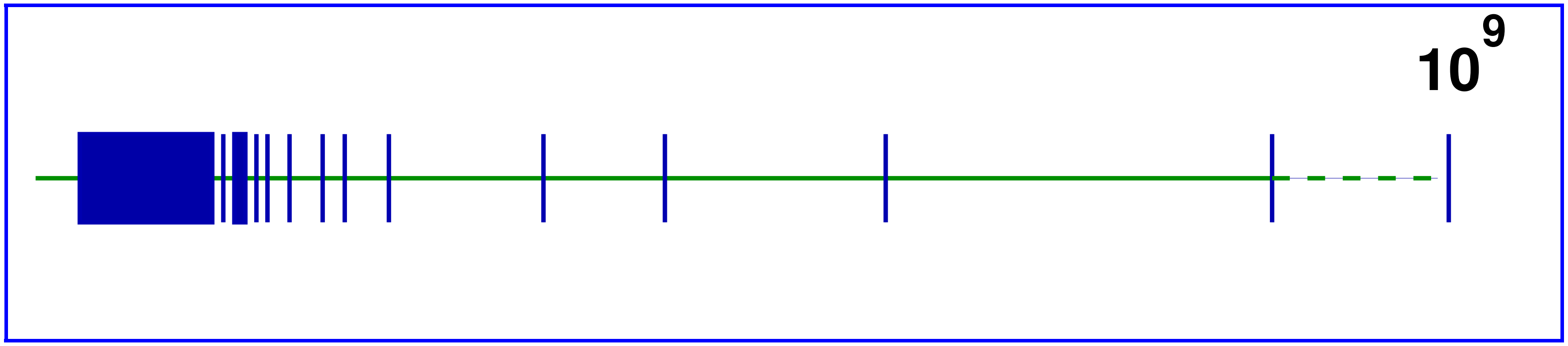
➤ We must have:

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

RATIONAL FILTERS

Why use rational filters?

➤ Consider a spectrum like this one:



➤ Polynomial filtering utterly ineffective for this case

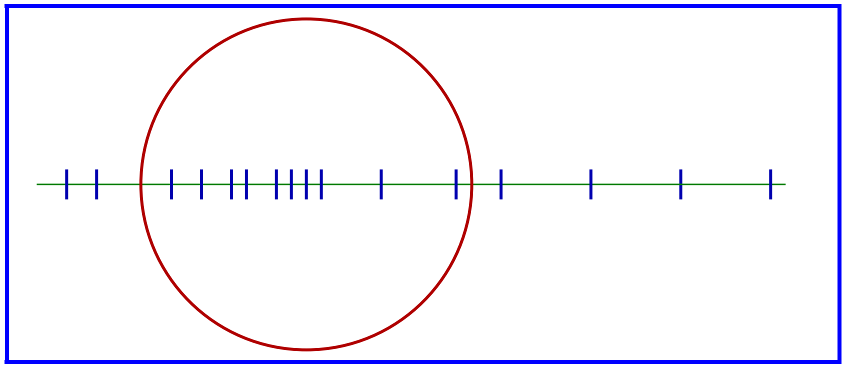
➤ Second issue: situation when Matrix-vector products are expensive

➤ 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



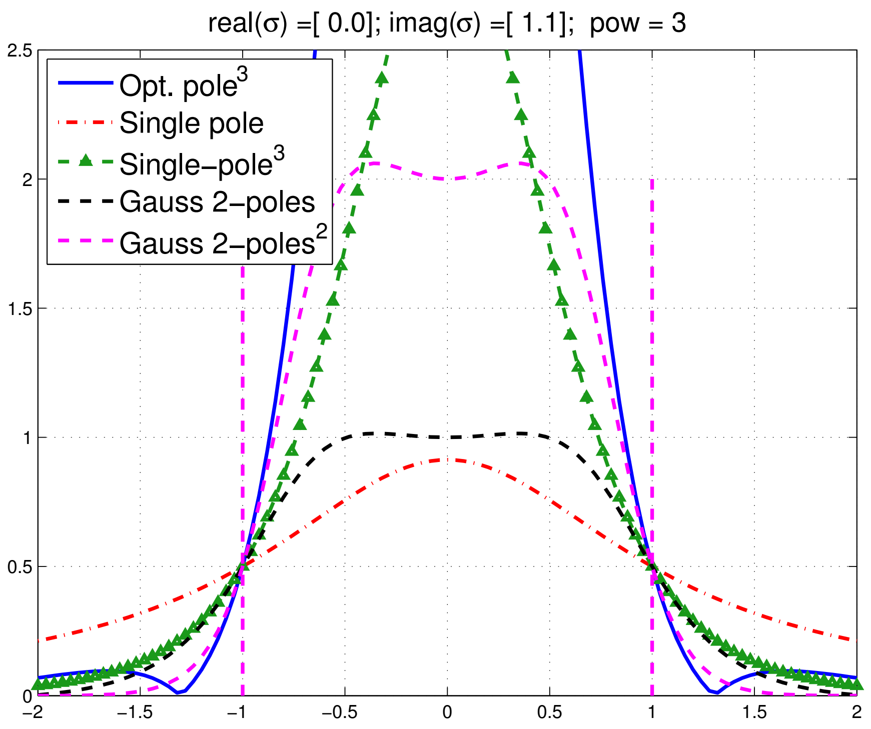
$P = \frac{-1}{2i\pi} \int_\Gamma (A - sI)^{-1} ds$

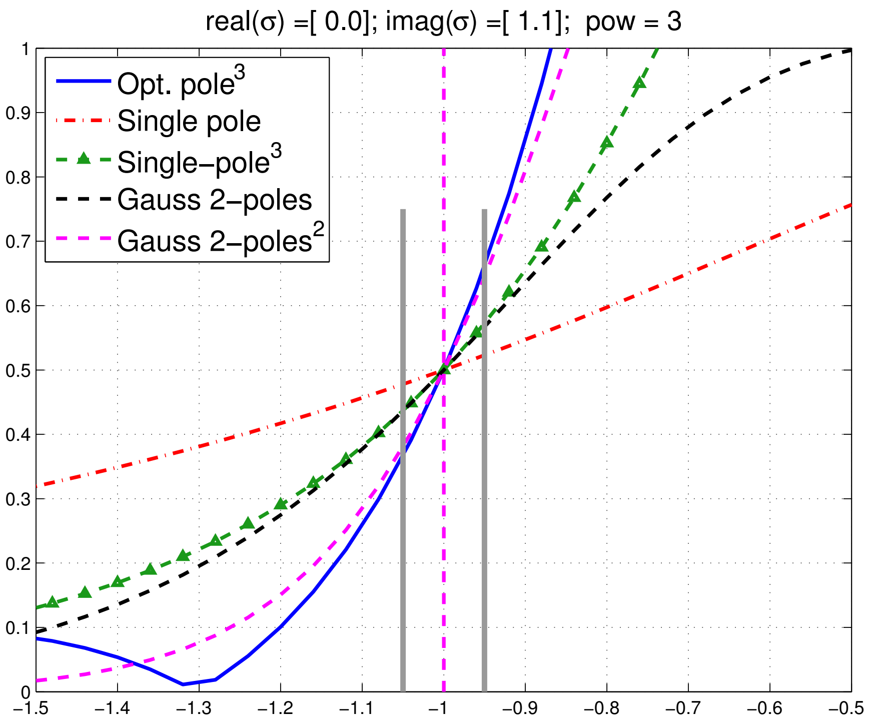
- Numer. integr. $P \rightarrow \tilde{P}$
- Use Krylov or S.I. on $\tilde{P}$

➤ Sakurai-Sugiura approach [Krylov]

➤ Polizzi [FEAST, Subsp. Iter.]

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

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

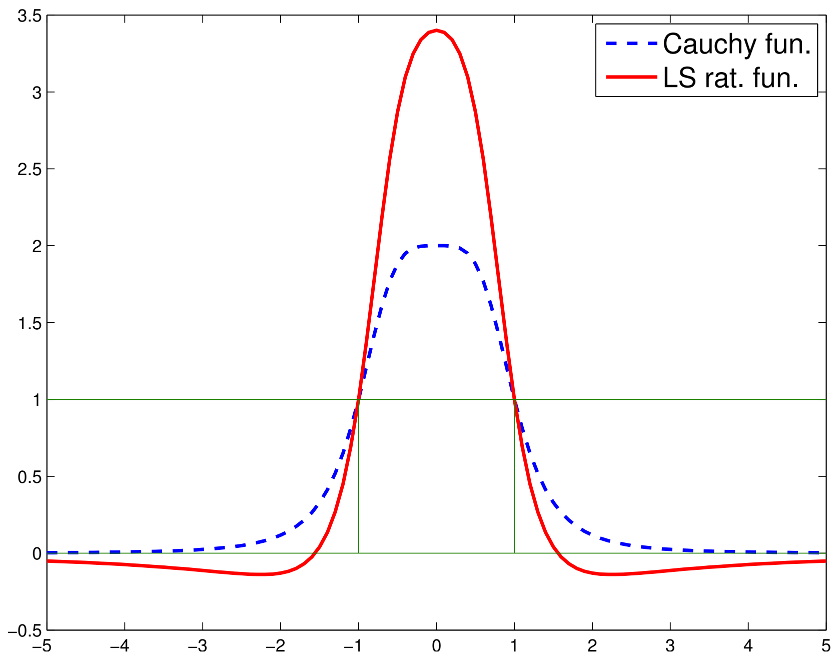
- $h(t)$ = step function $\chi_{[-1,1]}$.
- $w(t)$= weight function.

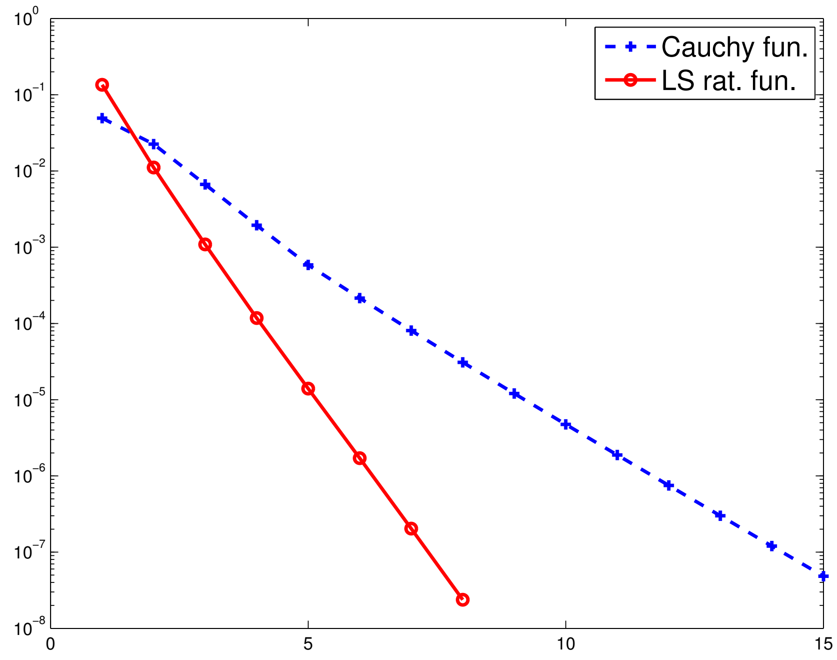
For example $a = 10$, $\beta = 0.2$

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

How does this work?

- Small example : Laplacean on a $\mathbf{43 \times 53}$ grid. ($\boldsymbol{n = 2279}$)
- 4 poles obtained from mid-point rule
- Want: all $(\boldsymbol{nev = 31})$ eigenvalues in $[\mathbf{0,\ 0.2}]$
- Use 1) standard subspace iteration + Cauchy (FEAST) then 2) subspace iteration + LS Rat. Appox.





- LS Uses the same poles + same factorizations as Cauchy but
- ... much faster as expected from a look at the curves of the functions

- Other advantages:

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

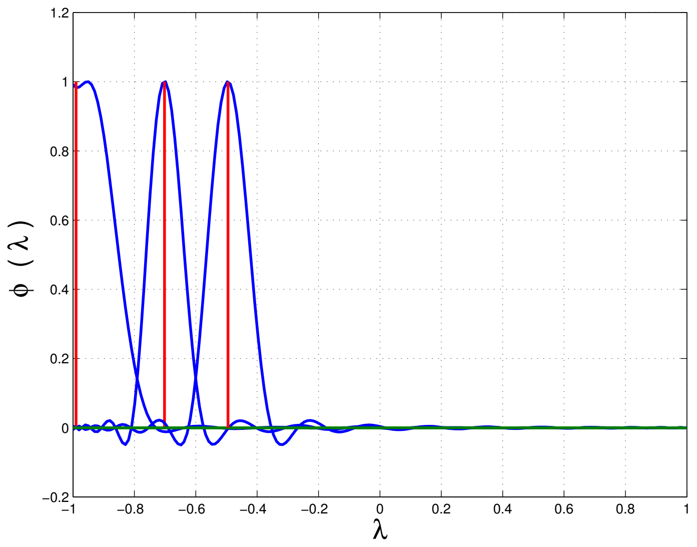
- Implemented in EVSL.. [Interfaced to UMFPACK as a solver]

*Spectrum Slicing and the **EVSL** project*

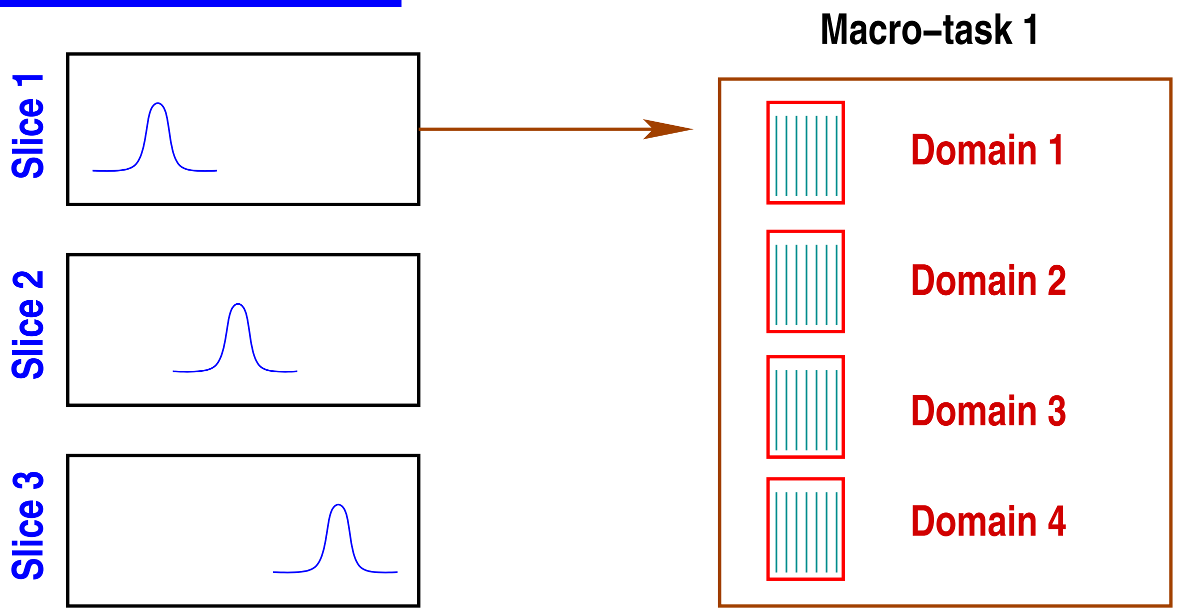
➤ EVSL package now at version 1.1.x

➤ Uses polynomial and rational filtering: Each can be appealing in different situations.

Spectrum slicing: Invokes Kernel Polynomial Method or Lanczos quadrature to cut the overall interval containing the spectrum into small sub-intervals.

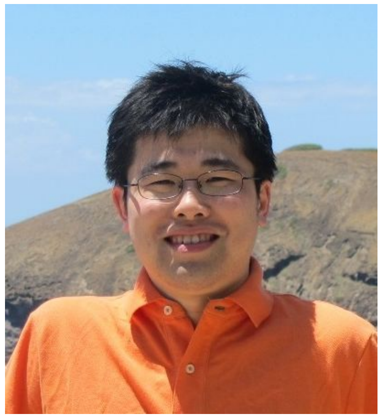


Levels of parallelism



The two main levels of parallelism in EVSL

EVSL Main Contributors (version 1.1.0+) & Support



- Ruipeng Li
LLNL

- Yuanzhe Xi
Asst. Prof. Emory

- Luke Erlandson
PhD Student, GTech.

➤ Work supported by NSF (past work: DOE)

➤ See web-site for details:

`http://www-users.cs.umn.edu/~saad/software/EVSL/`

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 Released back in August 2017.

- 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 pEVSL – In progress

- Fully parallel version [MPI + openMP]

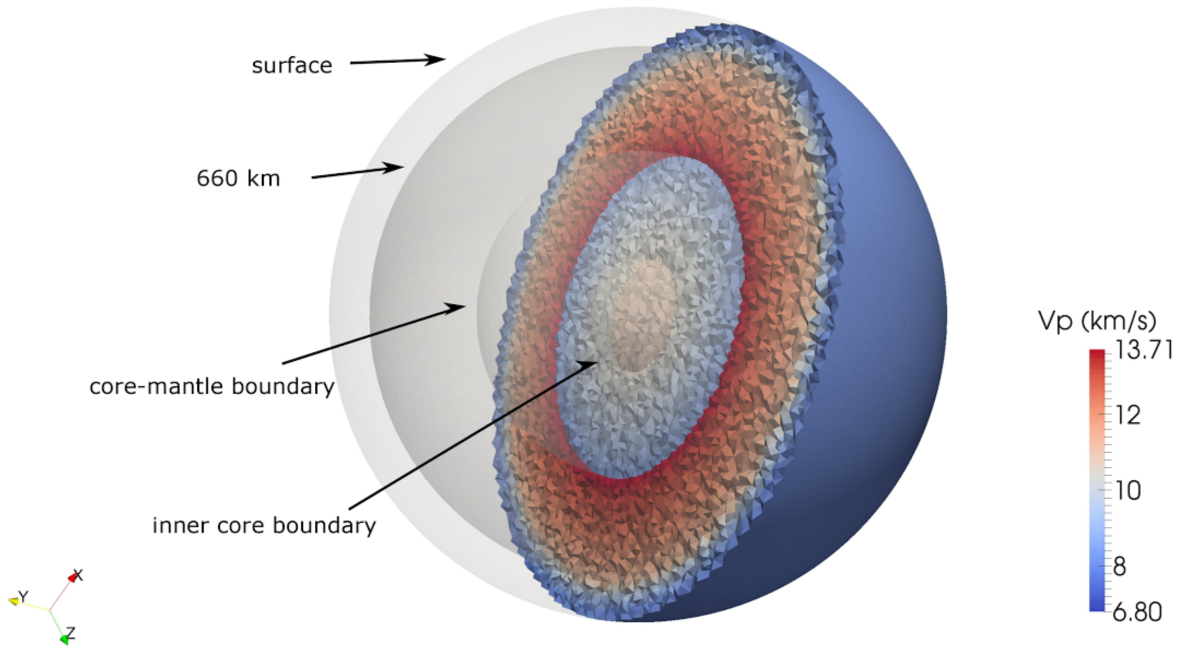
Spectrum slicing and the EVSL package

- All eigenvalues in $[\mathbf{0},\ \mathbf{1}]$ of of a $\mathbf{49^3}$ discretized Laplacian
- eigs(A,1971,'sa'): 14830.66 sec
- Solution: Use DOS to partition $[\mathbf{0},\ \mathbf{1}]$ into 5 slices
- Polynomial filtering from EVSL on Mesabi MSI, 23 threads/slice

$[\boldsymbol{a_i}, \boldsymbol{a_{i+1}}]$	# eigs	CPU time (sec)			max residual
		matvec	orth.	total	
$[\mathbf{0.00000, 0.37688}]$	386	1.31	18.26	28.66	$\mathbf{2.5 \times 10^{-14}}$
$[\mathbf{0.37688, 0.57428}]$	401	3.28	38.25	56.75	$\mathbf{8.7 \times 10^{-13}}$
$[\mathbf{0.57428, 0.73422}]$	399	4.69	36.47	56.73	$\mathbf{1.7 \times 10^{-12}}$
$[\mathbf{0.73422, 0.87389}]$	400	5.97	38.60	61.40	$\mathbf{6.6 \times 10^{-12}}$
$[\mathbf{0.87389, 1.00000}]$	385	6.84	36.16	59.45	$\mathbf{4.3 \times 10^{-12}}$

➤ Grand tot. = 263 s. Time for slicing the spectrum: 1.22 sec.

Computing the Earth normal modes



- Collaborative effort: Rice-UMN:
  J. Shi, R. Li, Y. Xi, YS, and M. V. De Hoop
- FEM model leads to a generalized eigenvalue problem:

$$\begin{bmatrix} A_s & & E_{fs} \\ & 0 & A_d \\ E_{fs}^T & A_d^T & A_p \end{bmatrix} \begin{bmatrix} u^s \\ u^f \\ p^e \end{bmatrix} = \omega^2 \begin{bmatrix} M_s & & \\ & M_f & \\ & & 0 \end{bmatrix} \begin{bmatrix} u^s \\ u^f \\ p^e \end{bmatrix}$$

- Want all eigen-values/vectors inside a given interval
- Issue 1: ‘mass’ matrix has a large null space..
- Issue 2: interior eigenvalue problem
- Solution for 1: change formulation of matrix problem [eliminate p^e ...]

➤ New formulation :

$$\underbrace{\left\{\begin{pmatrix} A_s & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} E_{fs} \\ A_d \end{pmatrix} A_p^{-1} \begin{pmatrix} E_{fs}^T & A_d^T \end{pmatrix}\right\}}_{\widehat{A}} \begin{pmatrix} u^s \\ u^f \end{pmatrix} =$$

$$\omega^2 \underbrace{\begin{pmatrix} M_s & 0 \\ 0 & M_f \end{pmatrix}}_{\widehat{M}} \begin{pmatrix} u^s \\ u^f \end{pmatrix}$$

➤ Use polynomial filtering – need to solve with $\widehat{M}$ but ...

● ... severe scaling problems if direct solvers are used

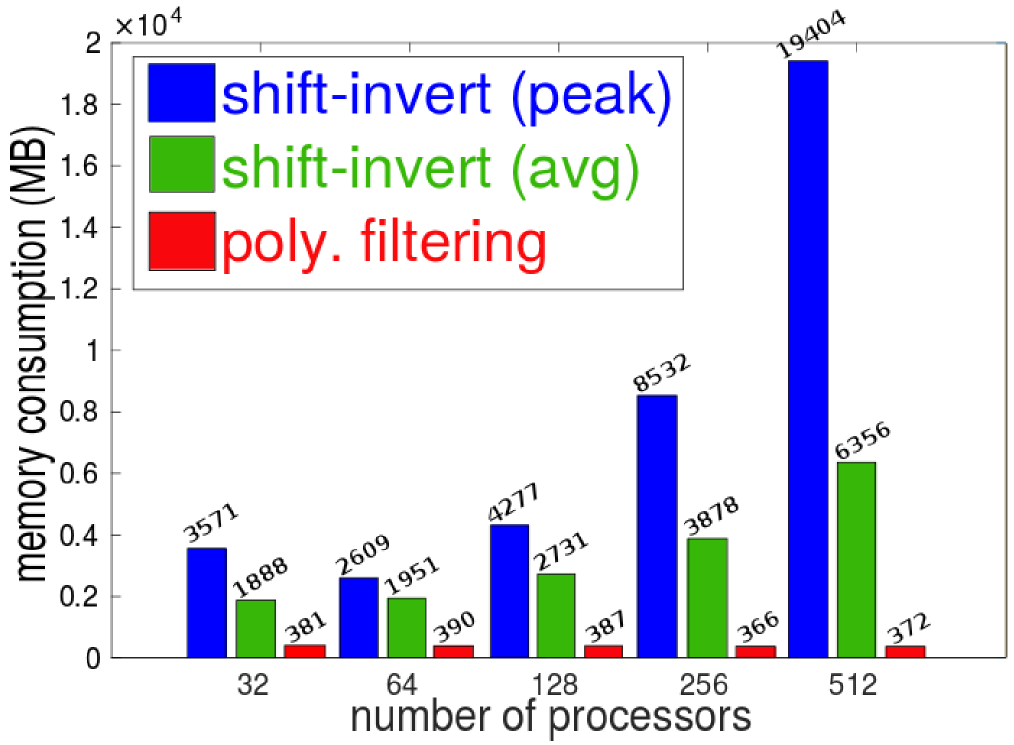
Hence:

➤ Replace action of M^{-1} by a low-deg. polynomial in M [to avoid direct solvers]

➤ Memory : parallel shift-invert and polynomial filtering

Machine: Comet, SDSC

Matrix size	# Proc.s
$591,303$	32
$1,157,131$	64
$2,425,349$	128
$4,778,004$	256
$9,037,671$	512



Recent: weak calability test for different solid (Mars-like) models on TACC Stampede2

nn/np	Mat-size	Av (ms)	$\leftarrow$ Eff.	Mv (ms)	$\leftarrow$ Eff.	$M^{-1}v$ (μs)	$\leftarrow$ Eff.
2/96	1,038,084	1760	1.0	495	1.0	0.01044	1.0
4/192	2,060,190	1819	0.960	568	0.865	0.0119	0.870
8/384	3,894,783	1741	0.948	571	0.813	0.0119	0.825
16/768	7,954,392	1758	0.959	621	0.763	0.0129	0.774
32/1536	15,809,076	1660	1.009	572	0.824	0.0119	0.834
64/3072	31,138,518	1582	1.043	566	0.820	0.0117	0.837
128/6144	61,381,362	1435	1.133	546	0.838	0.0113	0.851
256/12288	120,336,519	1359	1.173	592	0.757	0.01221	0.774

Nonlinear eigenvalue problems

- Joint work work with A. Miedlar and M. Elguide

$\boxed{T(z)u = 0}$ $z \to T(z)$ maps $\mathbb{C}$ to $\mathbb{C}^{n\times n}$

- Classical (well-understood) case: Polynomial:

$$T(z) = A_0 + zA_1 + \cdots + z^p A_p$$

- Often treated with linearization, e.g., when $p = 2$

$(A_0 + zA_1 + z^2 A_2)u = 0 \ \to$ (among other forms)

$$\left[\begin{pmatrix} 0 & I \\ -A_0 & -A_1 \end{pmatrix} - z\begin{pmatrix} I & 0 \\ 0 & A_2 \end{pmatrix}\right]\begin{pmatrix} u \\ zu \end{pmatrix} = 0$$

- General case can be very different from linear case.

Restrict slightly the class of problems we consider:

$$\boxed{T(z) = -B_0 + zA_0 + f_1(z)A_1 + \ldots + f_p(z)A_p}$$

- ➤ Main assumption: each of the analytic functions $f_j : \Omega \to \mathbb{C}$ well approximated by a rational function.
- ➤ Write (Cauchy integral representation of f_j):

$$f_j(z) = -\frac{1}{2i\pi}\int_\Gamma \frac{f_j(t)}{z-t}\,dt, \qquad z \in \Omega.$$

- ➤ Then use numerical quadrature with quadrature points σ_i's on contour $\Gamma \to$

$$f_j(z) \approx r_j(z) \equiv \sum_{i=1}^{m} \frac{\alpha_{ij}}{z-\sigma_i}.$$

- Consequence: $T(z)$ approximated by

$$\tilde{T}(z) = -B_0 + zA_0 + \sum_{j=1}^{p}\sum_{i=1}^{m} \frac{\alpha_{ij}}{z-\sigma_i} A_j = \dots$$

$$\equiv \; -B_0 + zA_0 + \sum_{i=1}^{m} \frac{B_i}{z-\sigma_i}, \qquad \text{where:}$$

$$B_i = \sum_{j=0}^{p} \alpha_{ij} A_j, \qquad i = 1, \dots, m.$$

$$\boxed{\left[-B_0 + zA_0 + \sum_{i=1}^{m} \frac{B_i}{z-\sigma_i}\right] u = 0}$$

- 'Surrogate' for original problem $T(z)u = 0$

Linearization

$$v_i = \frac{u}{\sigma_i - z} \rightarrow \tilde{T}(z)u = (-B_0 + zA_0)u - \sum_{i=1}^{m} B_i v_i,$$

- $\tilde{T}(\lambda)u = 0$ iff $\boxed{\mathcal{A}w = \lambda \mathcal{M}w}$ where:

$$\mathcal{M} = \begin{bmatrix} I & & & & \\ & I & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & A_0 \end{bmatrix}, \qquad \mathcal{A} = \begin{bmatrix} \sigma_1 I & & & & -I \\ & \sigma_2 I & & & -I \\ & & \ddots & & \vdots \\ & & & \sigma_m I & -I \\ B_1 & B_2 & \dots & B_m & B_0 \end{bmatrix}.$$

- Eigenvalue problem of size $n(m+1)$
- Special form: matrix need not be stored explicitly.

Approaches

1. Can use a shift-and-invert Arnlodi on whole system [Pb: memory when $m >> 1$]

➤ Block structure exploited.

2. Can use a shift-and-invert Subspace iteration [memory: similar pb.]

➤ Advantages: Less memory, ‘one-shot-method’ can be very efficient (memory)

3. Add restart to 2 but work only with vectors of length n.

Reduced Subspace Iteration: (Case when $\mathcal{M} = I$)

```
1. While Convergence not yet reached
2.     For $j = 1 : \nu$
3.         Select $w = [v;\ u]$                // See below
4.         Do $q$ steps of inverse iteration: $w := (\mathcal{A} - \sigma I)^{-1} w$
5.         If $w = [v;\ u] \equiv$ last iterate, set $U(:, j) = u$
6.     EndFor
7.     Use $U$ to perform Rayleigh-Ritz procedure
8. EndWhile
```

Step 2: (1) Very first outer loop: take random vectors.
(2) Other outer iterations: If (λ, u) is an eigenpair from step 7, define v-part as $v_i = u/(\sigma_i - \lambda)$ - then:

$$w = [v_1;\ v_2;\ \cdots\ ;\ v_m;\ u] \quad \text{(Matlab notation)}$$

Accuracy of computed eigenvalues

Proposition Let us assume that $\|f_j(z) - r_j(z)\|_{\Omega_1} \leq \varepsilon$ for $j = 1, \cdots, p$ and let $(\widetilde{\lambda}, \widetilde{u})$ be an exact eigenpair of the surrogate problem with $\widetilde{\lambda}$ located inside Ω_1 and $\|\widetilde{u}\| = 1$ for a certain vector norm $\|\cdot\|$. Let $\mu = \sum_{j=1}^{p} \|A_j\|$. Then,

$$\|T(\widetilde{\lambda})\widetilde{u}\| \leq \mu\varepsilon.$$

Proposition Let us assume that $\|f_j(z) - r_j(z)\|_{\Omega_1} \leq \epsilon$ for $j = 1, \cdots, p$ and let (λ, u) be an exact eigenpair for $T(z)$ with λ located inside Ω_1 and $\|u\| = 1$. Then, (λ, u) is an approximate eigenpair of the surrogate problem, i.e.,

$$\|\widetilde{T}(\lambda)u\| \leq \mu\varepsilon,$$

where μ is defined above.

The halo of extraneous eigenvalues

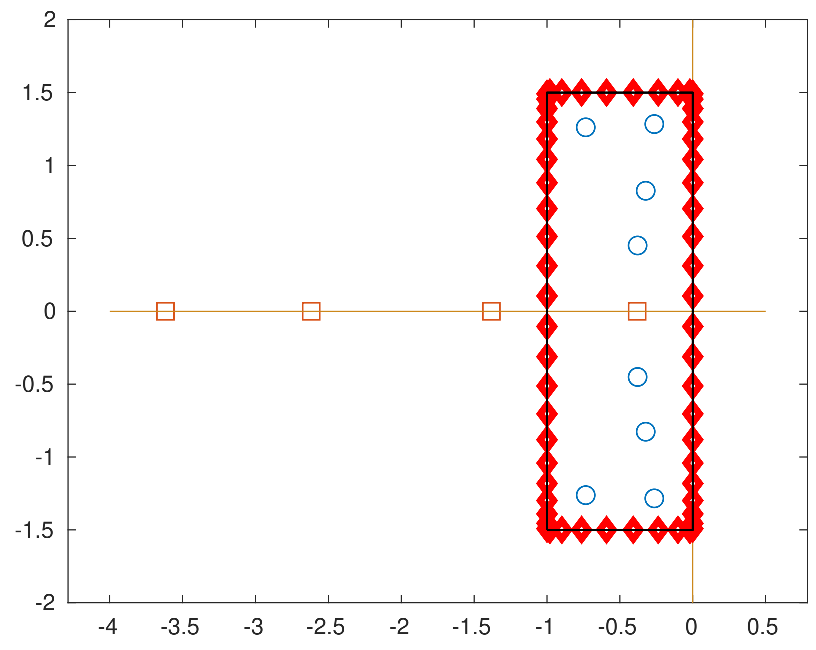
➤ Observed behavior: many ‘extraneous’ or ‘spurious’ eigenvalues congregate around the contour of integration..

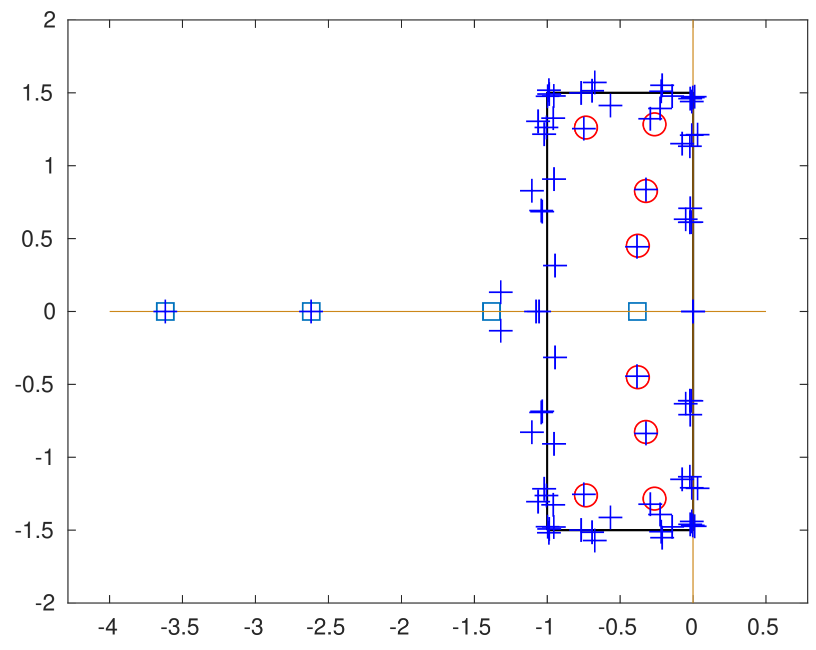
Example: $T(z) = -B_0 + \lambda A_0 + \lambda^2 A_2$ where [Matlab] (n=4)

```
B0=-2*eye(n)+diag(ones(n-1,1),1)+diag(ones(n-1,1),-1);
A0=eye(n);
A2=0.5*(n*eye(n)-eye(n,1)*ones(1,n)-ones(n,1)*eye(1,n));
```

➤ Spectrum inside rectangle with bottom-left and top-right corners $(-1, -1.5i), (0, 1.5i)$

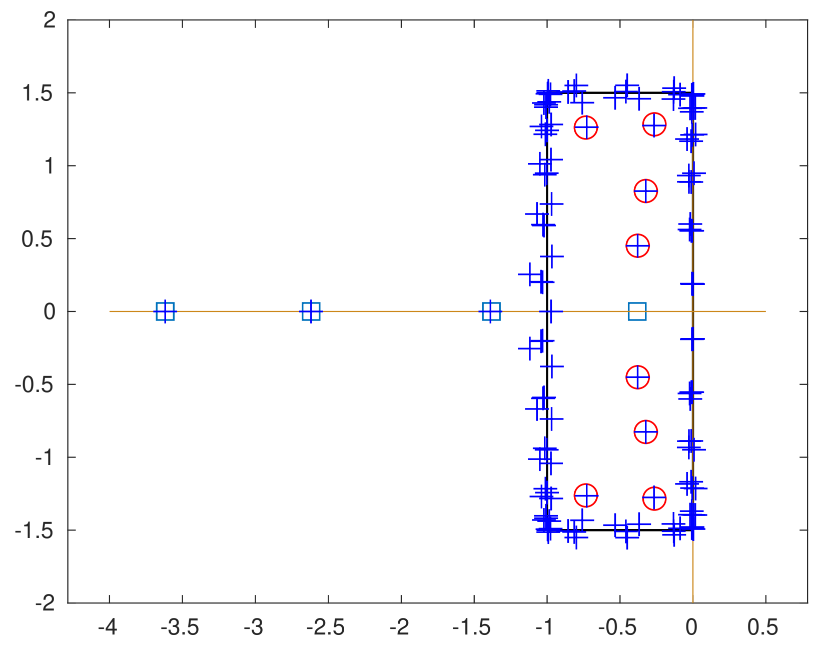
➤ Use this for integration contour.

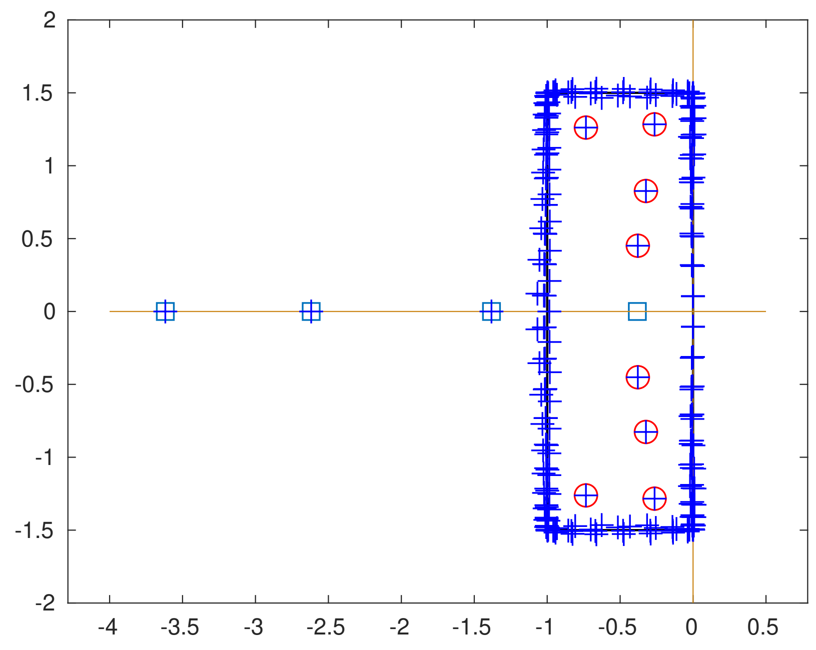




Left: The 8 eigenvalues of original problem (circle); the 4 eigenvalues of the linear part (square); contour and quadrature points along it.

Right: Eigenvalues computed with $m = 20$ quadrature points (plus) along with contour, original eigenvalues (circle), and eigen-values of linear part (square).





Using a total of $m = 32$ quadrature points (left) and $m = 60$ quadrature points (right).

(i) Spectrum of Linear part outside contour *APPROXIMATED*
(ii) Spectrum of Linear part inside contour *IGNORED*
(iii) Spectrum of $T(z)$ inside contour *APPROXIMATED*
(iv) Other eigenvalues populate the contour

Example

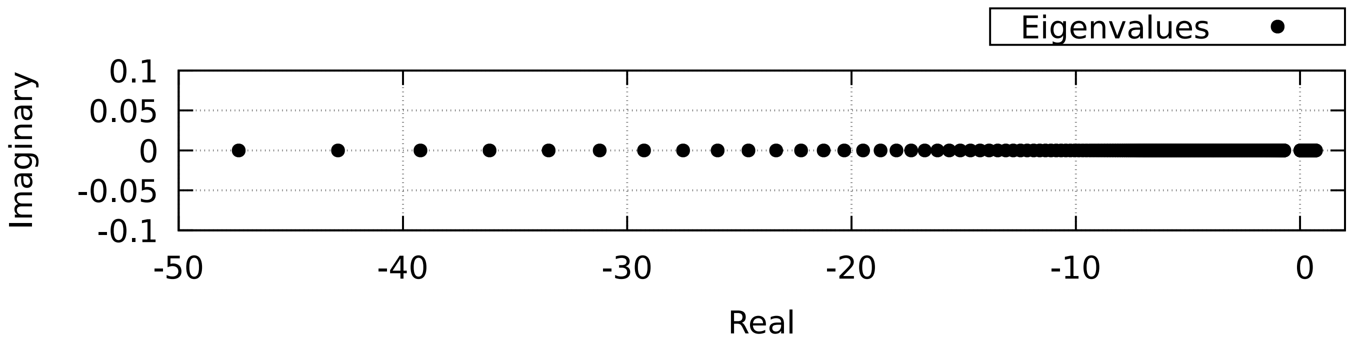
Hadeler problem of dimension $n = 200$:

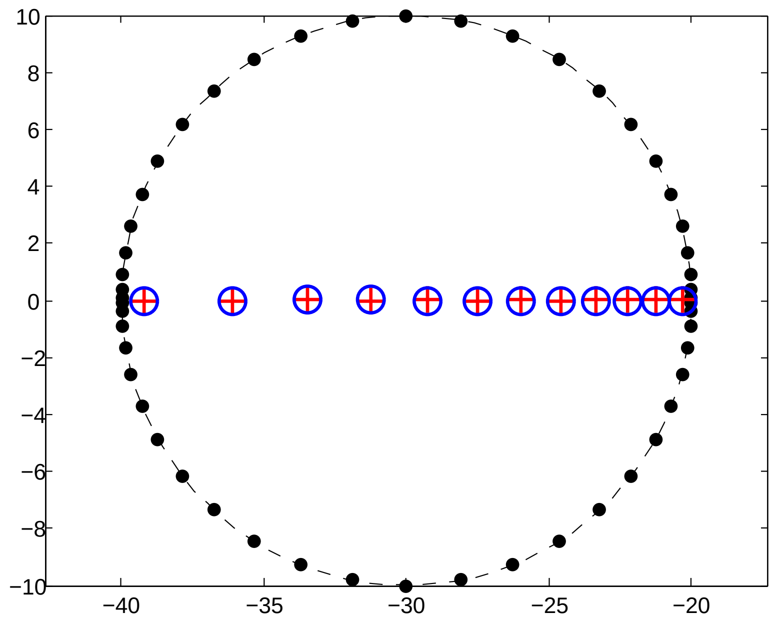
$$T(\lambda) = (e^{\lambda} - 1)B_1 + \lambda^2 B_2 - B_0 \quad \text{with:}$$

$$B_0 = b_0 I, \quad b_0 = 100$$

$$b_{jk}^{(1)} = (n + 1 - \max(j,k))jk,$$

$$b_{jk}^{(2)} = n\delta_{jk} + 1/(j+k),$$





Eigenvalues of Hadeler Pb. inside a circle of radius $\boldsymbol{r = 10}$ and center $\boldsymbol{c = -30}$ obtained by the reduced subspace iteration ('+'), and by Beyn's method ('O'). Quadrature: Gauss-Legendre with 50 points.

➤ Current work: Helmholtz equation (in 3-D):

$$\boldsymbol{\Delta u + k^2 u = 0 \quad + B.C.}$$

Using the Boundary Element Method (BEM) produces a nonlinear eigenvalue problem.

Conclusion

- EVSL code available here: [Current version: version 1.1.1]

  $\boxed{\texttt{www.cs.umn.edu/~saad/software/EVSL}}$

- EVSL Also on github (development)

Plans: (1) Release fully parallel code; (2) Block versions; (3) Iterative solvers for rational filt.; (4) Nonhermitian case;

- Earth modes calculations done with fully parallel code
- Scalability issues with parallel direct solvers ...
- ... Needed: iterative solvers for the highly indefinite case
- Frontier in eigenvalue problem: *Nonlinear* case