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Divide and conquer algorithms for large eigenvalue problems

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Collaborators:

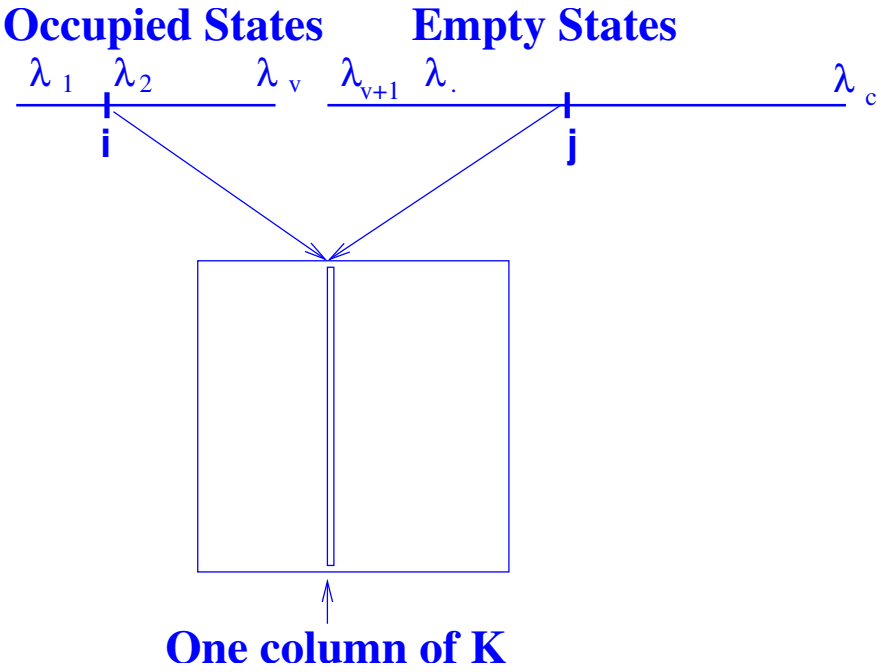
- Joint work with
  - Vassileos Kalantzis [grad student]
  - Ruipeng Li [grad student]
  - Haw-ren Fang [former post-doc]
  - Grady Schoefield and Jim Chelikowsky [UT Austin] [windowing into PARSEC]
- Work supported by DOE : Scalable Computational Tools for Discovery and Design: Excited State Phenomena in Energy Materials [Involves 3 institutions: UT Austin, UC Berkeley, U Minn]

Introduction & Motivation

- Density Functional Theory deals with ground states
- Excited states involve transitions and invariably lead to much more complex computations
- Problem: very large number of eigenpairs to compute

An illustration: Time-Dependent Density Functional Theory (TDDFT). In the so-called Cassida approach we need to compute the eigenvalues of a dense matrix $\boldsymbol{K}$ which is built using both occupied and unocuppied states

- Each pair $\longrightarrow$ one column of K
- To compute each column need to solve a Poisson eqn. on domain
- Intense calculation , lots of parallelism



An illustration: Si34 H36 [Done in 2004-2005]

- Number of Occupied States (Valence band) $n_v = 86$
- Number of Unoccupied States (Conduction band) $n_c = 154$
- Size of Coupling Matrix: $N = n_v * n_c = 13,244$
- Number of Poisson solves = 13,244

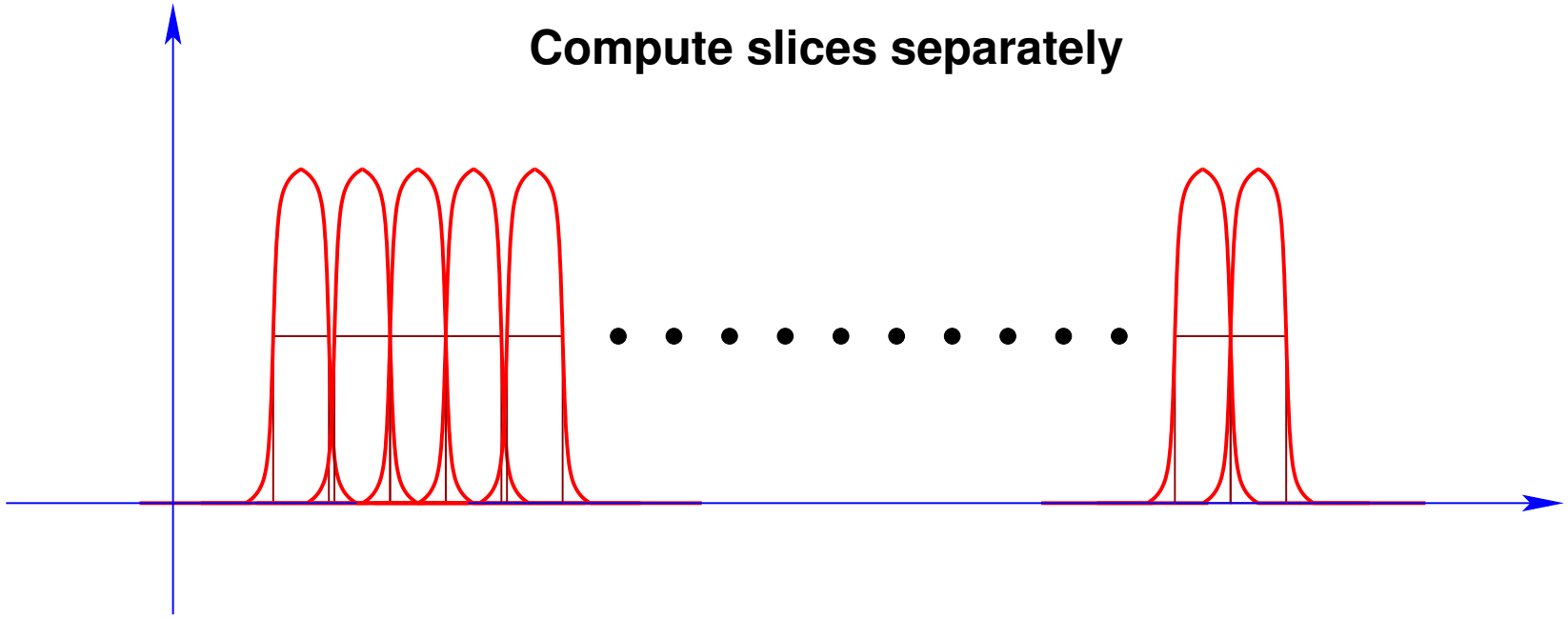
- Similar types of calculations in the GW approach [see, e.g., BerkeleyGW]
- But more complex
- Challenge:

'Hamiltonian of size $\sim$ 1 Million, get 10% of bands'

Solution: Spectrum Slicing

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



- Deceivingly simple looking idea.
- Issues:
  - Deal with interfaces : duplicate/missing eigenvalues
  - Window size [need estimate of eigenvalues]
  - How to compute each slice? [polynomial / rational filters?, ..]

Computing a slice of the spectrum

Q: How to compute eigenvalues in the middle of the spectrum of a large Hermitian matrix?

A: Common practice: Shift and invert + some projection process (Lanczos, subspace iteration..)

Main steps:

1) Select a shift (or sequence of shifts) σ;
2) Factor $A - \sigma I$: $A - \sigma I = LDL^T$
3) Apply Lanczos algorithm to $(A - \sigma I)^{-1}$

- Solves with $A - \sigma I$ carried out using factorization
- Limitation: factorization
- First Alternative: Polynomial filtering

POLYNOMIAL FILTERS

Polynomial filtering

- Apply Lanczos or Subspace iteration to: $M = \phi(A)$ 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
- Consider Subspace Iteration. In following script:
  - $B = (A - cI)/h$ so $\Lambda(B) \subset [-1,\ 1]$
  - Rayleigh-Ritz with B [shifted-scaled A]
  - Compute residuals w.r.t. B
  - Exit when enough eigenpairs have converged

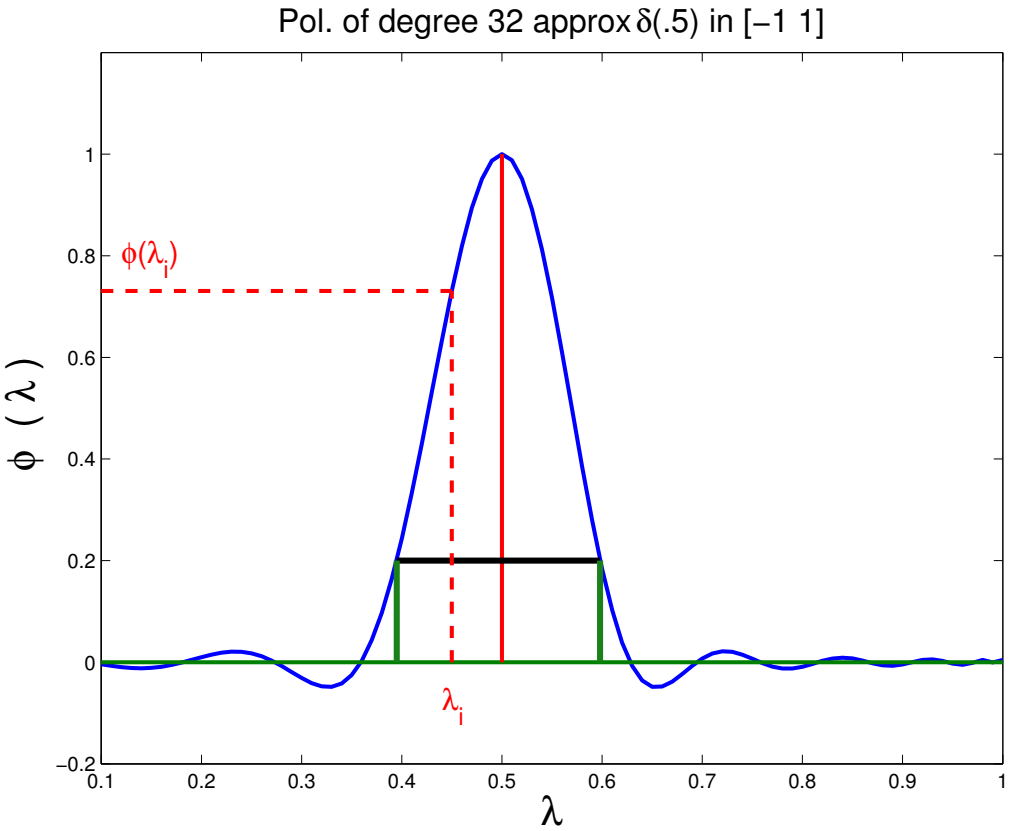
```
for iter=1:maxit
      Y = PolFilt(B, V, mu);
      [V, R] = qr(Y,0);
%— Rayleigh-Ritz with B
      C = V'*(B*V);
      [X, D] = eig(C);
      d = diag(D);
%— get e-values closest to center of interval
      [~, idx] = sort(abs(d-gam),'ascend');
%— get their residuals
      ...
%— if enough pairs have converged exit
      ...
end
```

What polynomials?

- For end-intervals can just use Chebyshev
- For inside intervals: several choices

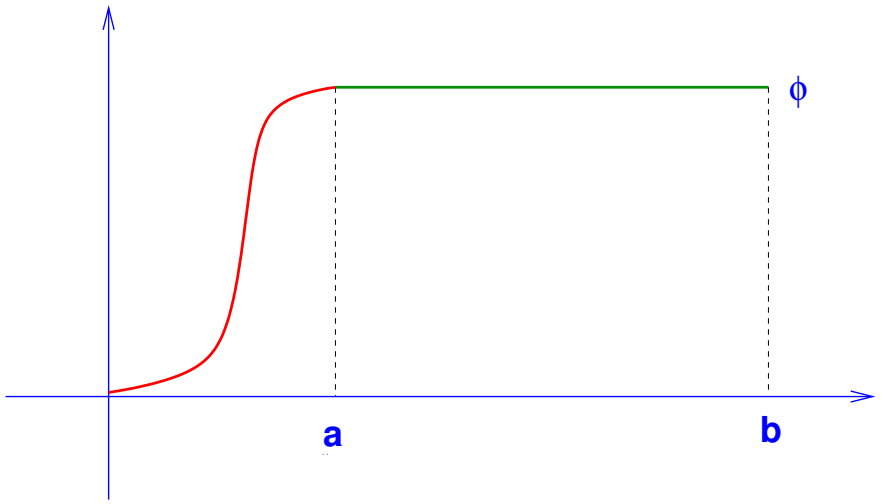
- Recall the main goal:

A polynomial that has large values for $\lambda \in [a, b]$ small values elsewhere



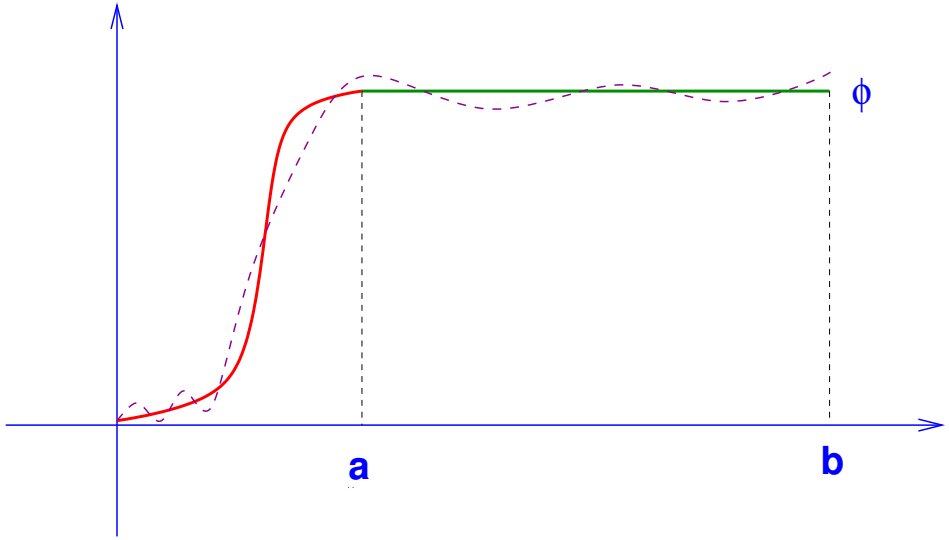
Least-squares approach

- Two stage approach used in filtlan [H-r Fang, YS 2011] -
- First select an "ideal filter"
- e.g., a piecewise polynomial function [a spline]



- For example $\phi =$ Hermite interpolating pol. in [0,a], and $\phi = 1$ in [a, b]
- Referred to as the 'Base filter'

- Then approximate base filter by degree k polynomial in a least-squares sense.
- Can do this without numerical integration

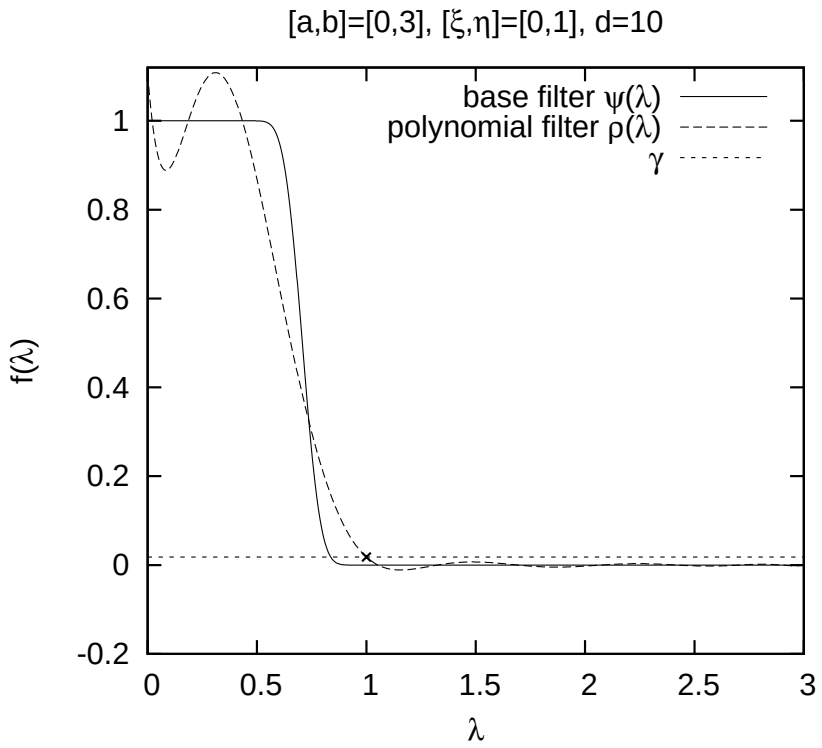


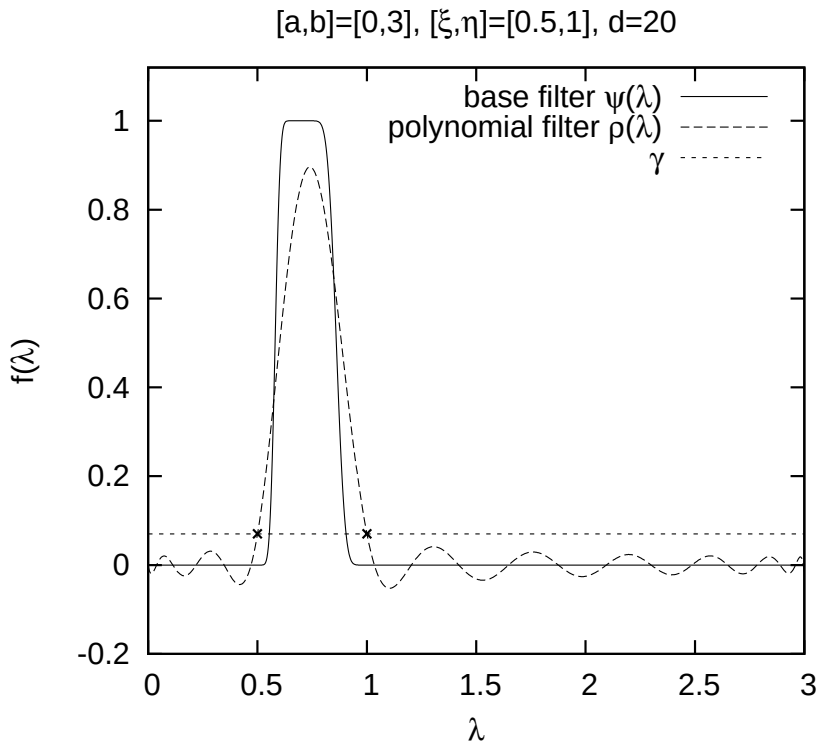
Main advantage: Extremely flexible.

Method: Build a sequence of polynomials ϕ_k which approximate the ideal PP filter ϕ, in the L_2 sense.

➤ In filtlan, we used a form of Conjugate Residual technique in polynomial space. Details skipped.

Low-pass, high-pass, & barrier (mid-pass) filters

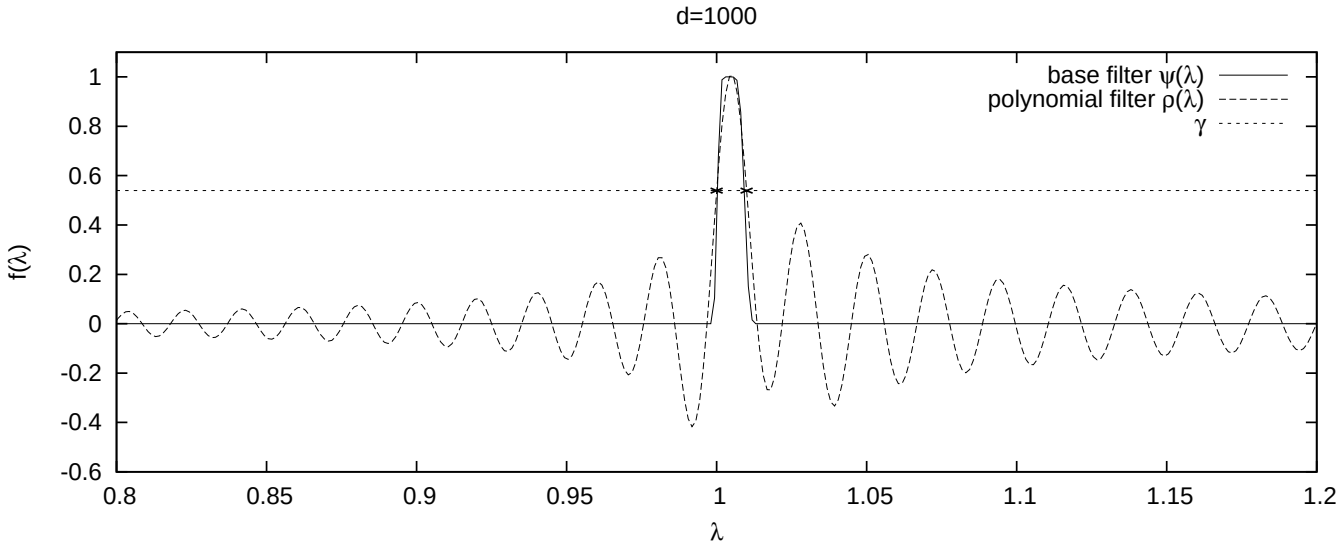




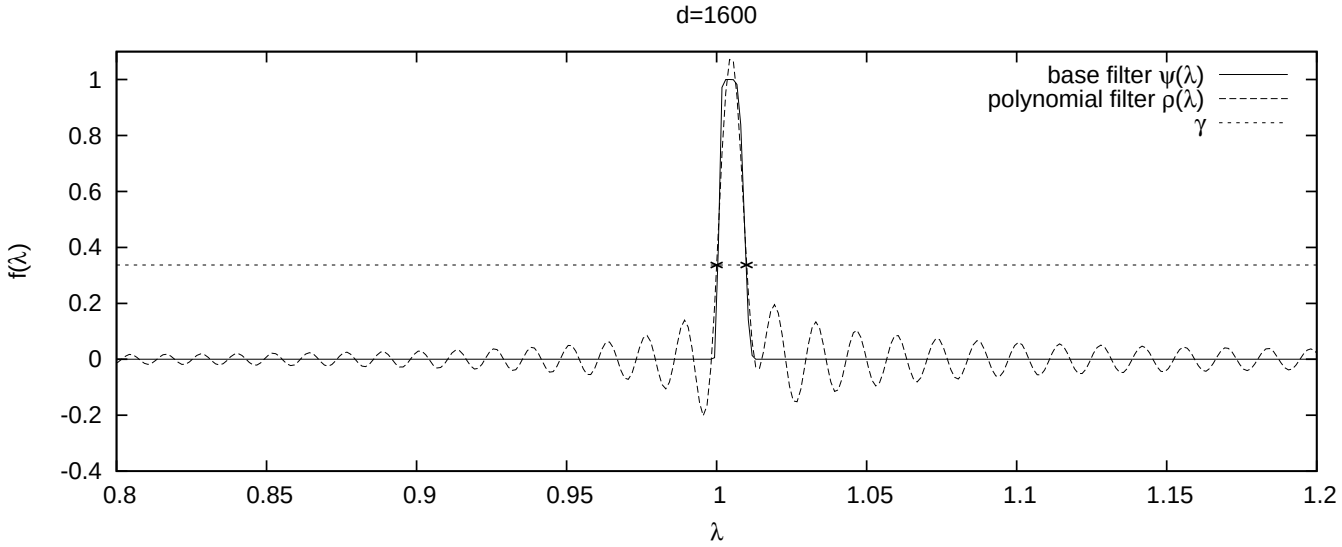
- See Reference on Lanczos + pol. filtering: Bekas, Kokiopoulou, YS (2008) for motivation, etc.
- H.-r Fang and YS "Filtlan" paper [SISC,2012] and code

Misconception: High degree polynomials are bad

Degree 1000 (zoom)



Degree 1600 (zoom)



A simpler approach: Chebyshev + Jackson damping

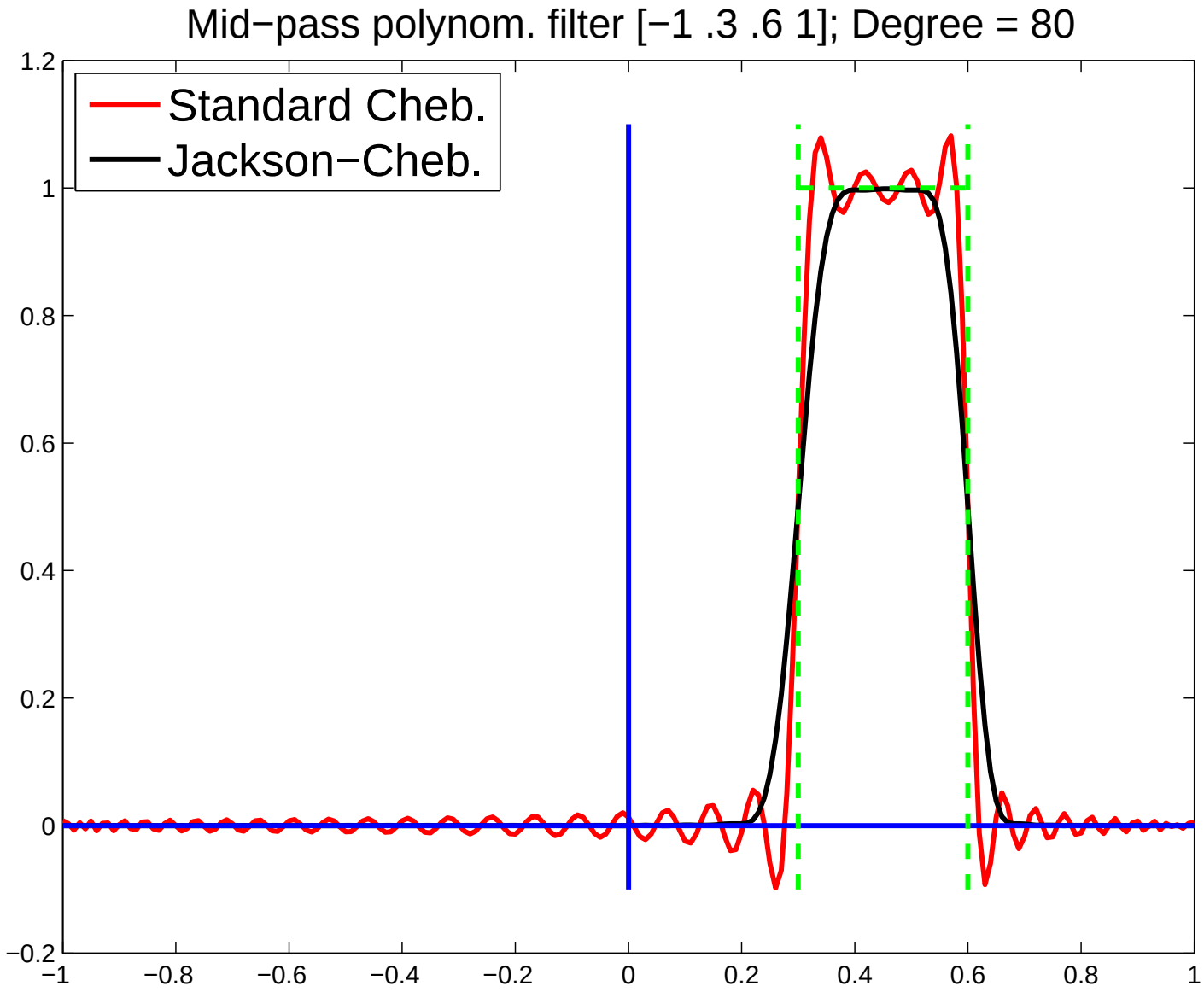
- Simply seek the best LS approximation to step function
- Add damping coefficients to reduce oscillations

Chebyshev-Jackson approximation of a function f:

$$f(x) \approx \sum_{i=0}^{k} g_i^k \gamma_i T_i(x)$$

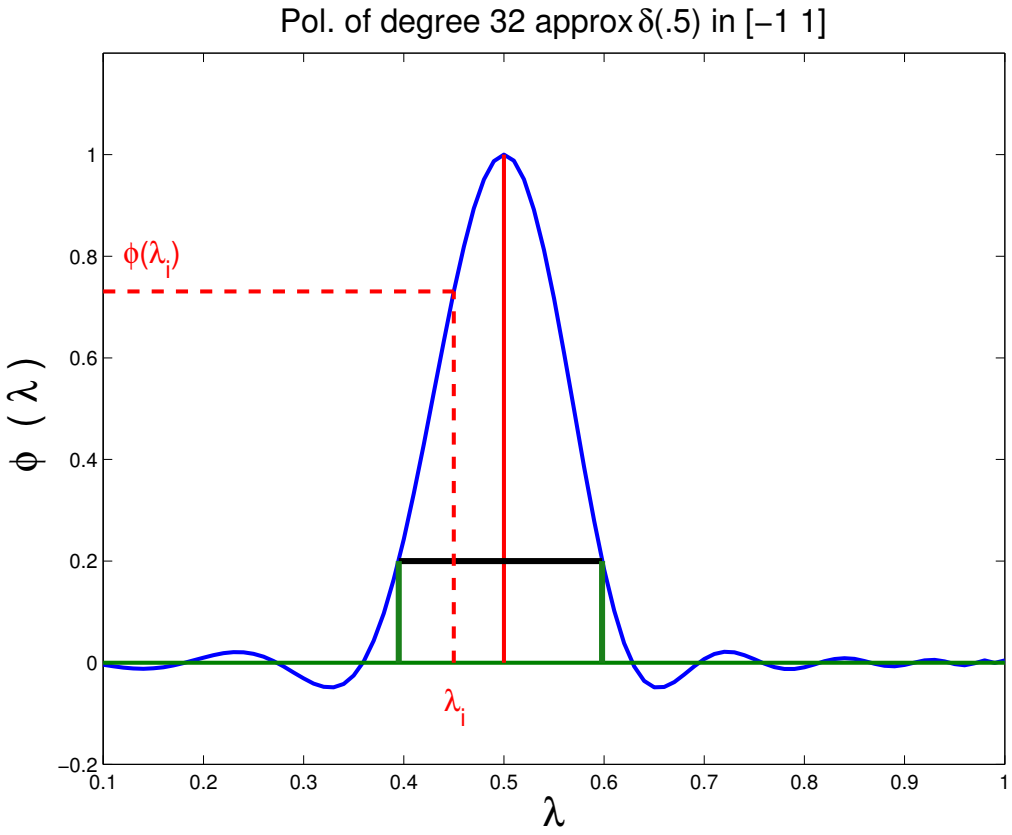
$$\gamma_i = \begin{cases} [\arccos(a) - \arccos(b)]/\pi : i = 0 \\ 2\,[\sin(i\arccos(a)) - \sin(i\arccos(b))]/(i\pi) : i > 0 \end{cases}$$

- Expression for g_i^k: see L. O. Jay, YS, J. R. Chelikowsky, '99

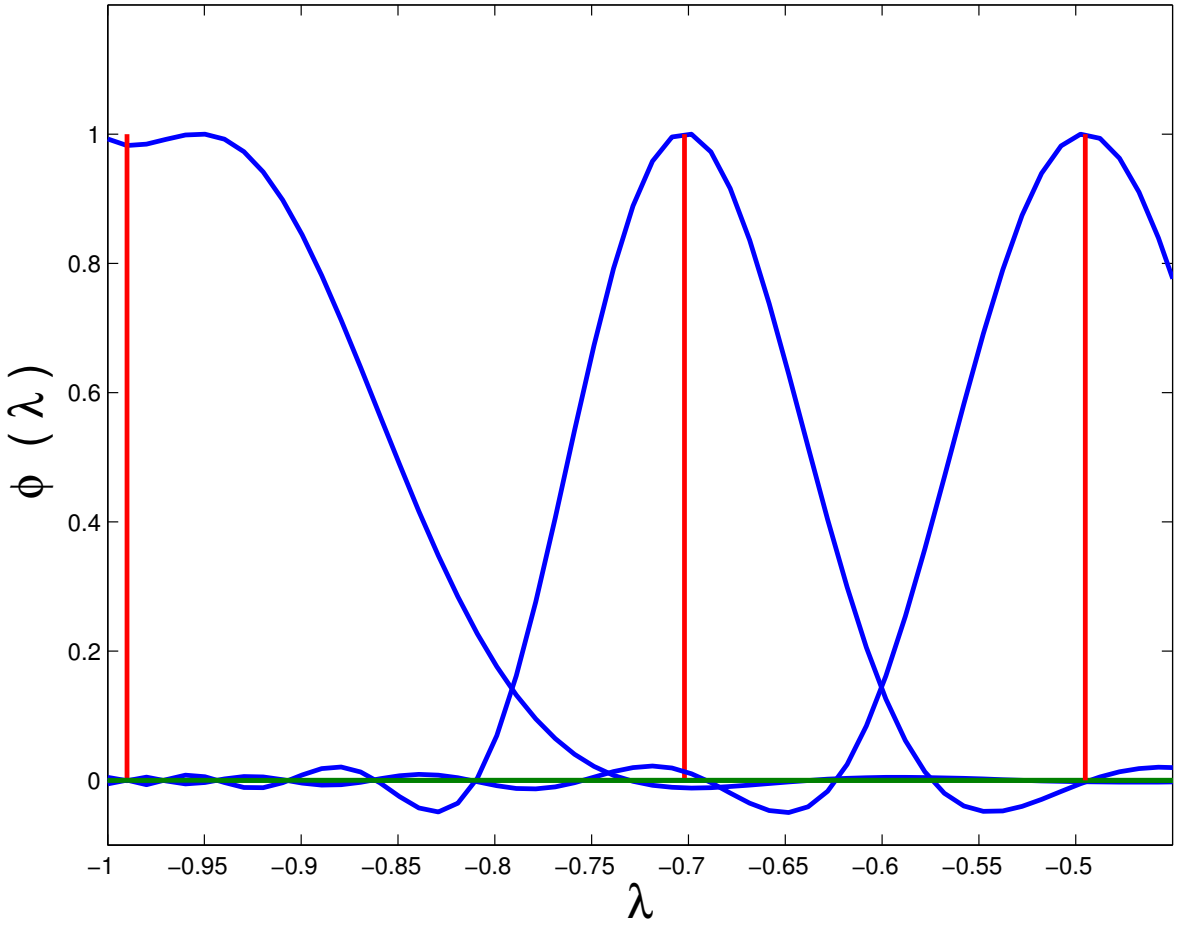

Mid−pass polynom. filter [−1 .3 .6 1]; Degree = 80
Standard Cheb.
Jackson−Cheb.
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1

Polynomial filters: An even simpler approach

- Simply seek the LS approximation to the δ – Dirac function
- Centered at the middle of the interval.
- Can use same damping: Jackson, or Lanczos σ damping.



Filters for 3 slices



Tests – Test matrices

** From Filtlan article with H-R Fang

➤ Experiments on two dual-core AMD Opteron(tm) Processors 2214 @ 2.2GHz and 16GB memory.

Test matrices:

* Five Hamiltonians from electronic structure calculations,

* `Andrews` matrix $N = 60,000$, $nnz \approx 760K$, interval $[4, 5]$; nev=1,844 eigenvalues, (3,751 to the left of η)

* A discretized Laplacian (FD) $n = 10^6$, interval = $[1,\ 1.01]$, nev= 276, (>17,000 on the left of η)

➤ Here : report only on Andrews and Laplacean

Results for Andrews - set 1 of stats

method	degree	# iter	# matvecs	memory
filt. Lan. (mid-pass)	$d = 20$	9,440	188,800	4,829
	$d = 30$	6,040	180,120	2,799
	$d = 50$	3,800	190,000	1,947
	$d = 100$	2,360	236,000	1,131
filt. Lan. (high-pass)	$d = 10$	5,990	59,900	2,799
	$d = 20$	4,780	95,600	2,334
	$d = 30$	4,360	130,800	2,334
	$d = 50$	4,690	234,500	2,334
Part. $\perp$ Lanczos		22,345	22,345	10,312
ARPACK		30,716	30,716	6,129

Results for Andrews - CPU times (sec.)

method	degree	$\rho(A)v$	reorth	eigvec	total
filt. Lan. (mid-pass)	$d = 20$	2,797	192	4,834	9,840
	$d = 30$	2,429	115	2,151	5,279
	$d = 50$	3,040	65	521	3,810
	$d = 100$	3,757	93	220	4,147
filt. Lan. (high-pass)	$d = 10$	1,152	2,911	2,391	7,050
	$d = 20$	1,335	1,718	1,472	4,874
	$d = 30$	1,806	1,218	1,274	4,576
	$d = 50$	3,187	1,032	1,383	5,918
Part. $\perp$ Lanczos		217	30,455	64,223	112,664
ARPACK		345	†423,492	†18,094	441,934

Results for Laplacian – Matvecs and Memory

method	degree	# iter	# matvecs	memory
	600	1,400	840,000	10,913
mid-pass filter	$1,000$	950	950,000	7,640
	$1,600$	710	1,136,000	6,358

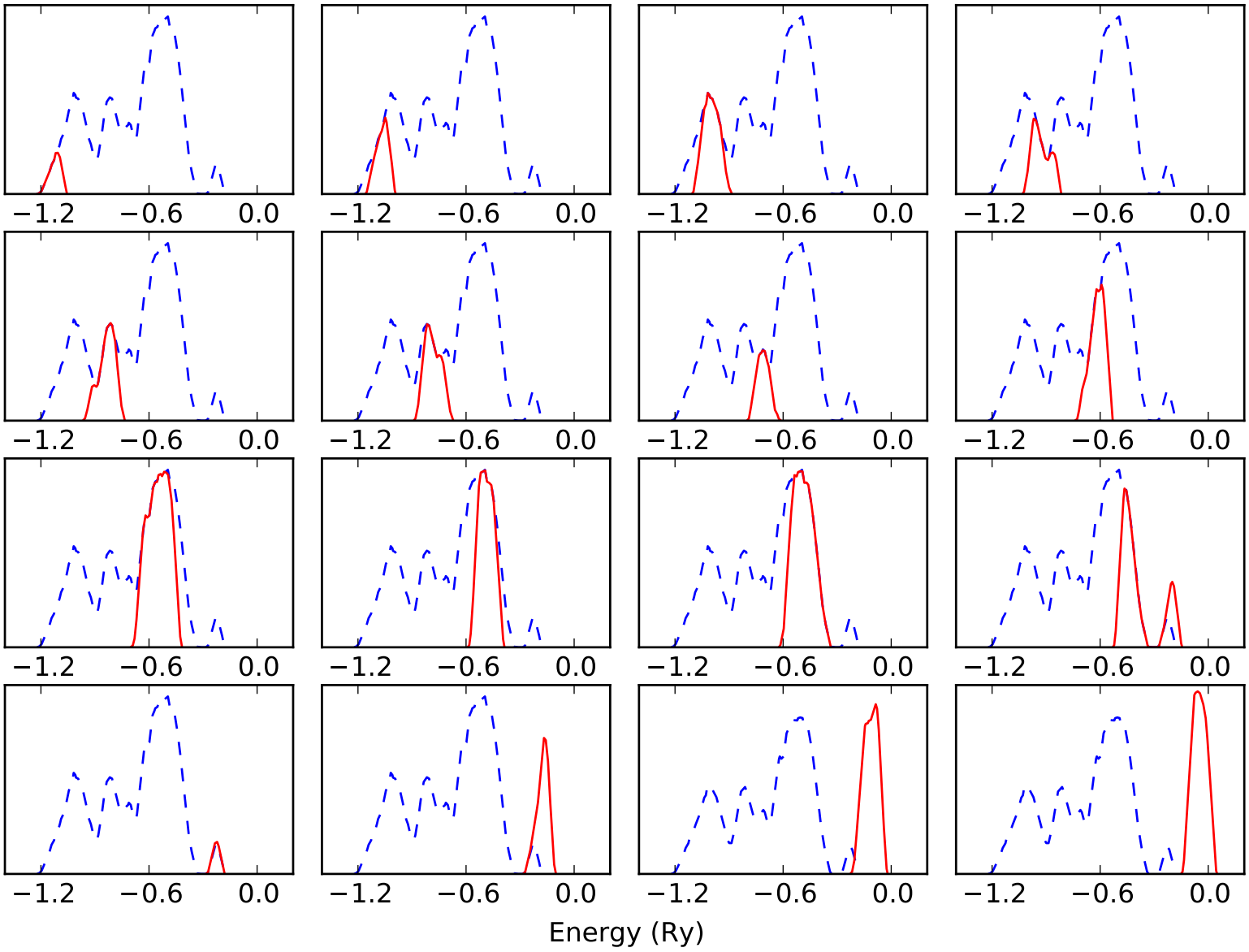
Results for Laplacian – CPU times

method	degree	$\rho(A)v$	reorth	eigvec	total
	600	97,817	927	241	99,279
mid-pass filter	$1,000$	119,242	773	162	120,384
	$1,600$	169,741	722	119	170,856

Spectrum slicing in PARSEC

** From: A Spectrum Slicing Method for the Kohn-Sham Problem, G. Schofield, J. R. Chelikowsky and YS, Computer Physics Comm., vol 183 (2011) pp. 487-505.

- Preliminary implementation in our code: *PARSEC*
- Uses the simpler Jackson-Chebyshev filters
- For details on windowing, etc., see paper
- Illustration shown next using 16 slices: *States for unrelaxed* $Si_{275}H_{172}$ *as computed using 16 slices. Each slice* $\rightarrow$ *solid line. Original full spectrum* $\rightarrow$ *dashed line.*

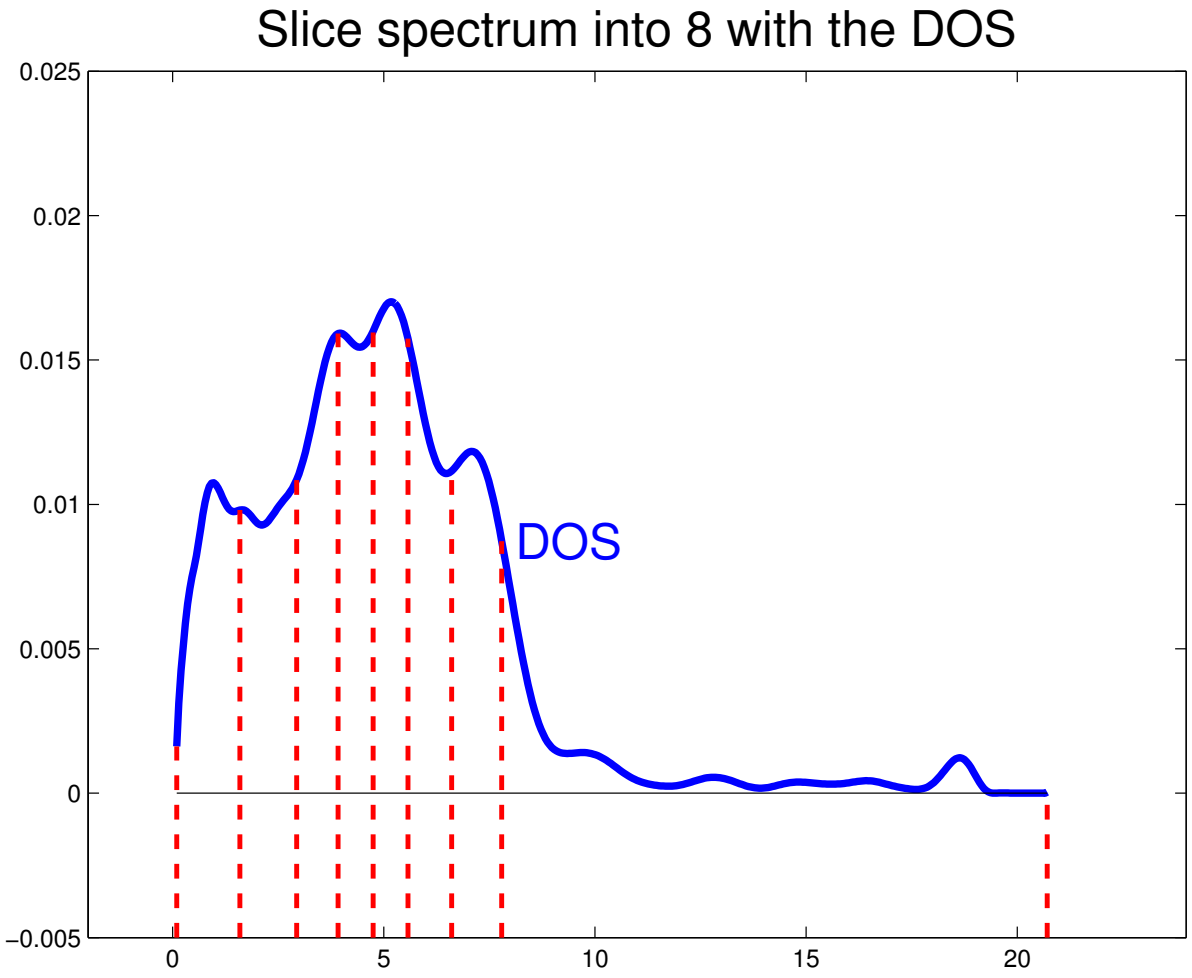

−1.2
−0.6
0.0
Energy (Ry)

How do I slice my spectrum?

Analogue question:

How would I slice an onion if I want each slice to have about the same mass?

- A good tool: Density of States – see:
  - L. Lin, YS, Chao Yang recent paper.
  - KPM method – see, e.g., : [Weisse, Wellein, Alvermann, Fehske, '06]
  - 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'
- Situation is much more complex



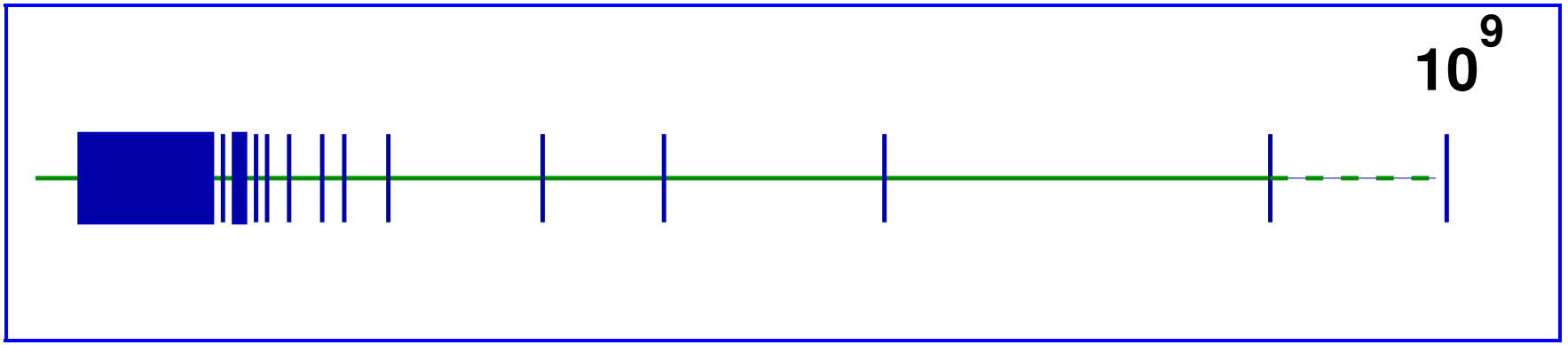
- We must have:

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

RATIONAL FILTERS

Why use rational filters?

- Consider a spectrum like this one:



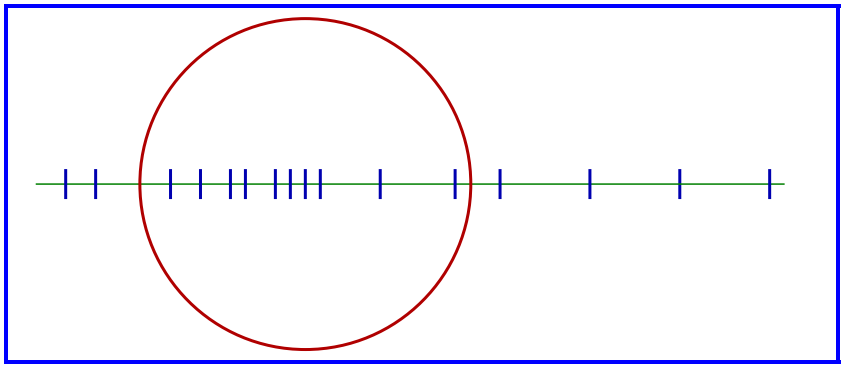
- Polynomial filtering approach would be utterly ineffective for this case

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

- Alternative is to use rational filters:

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

- 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.]

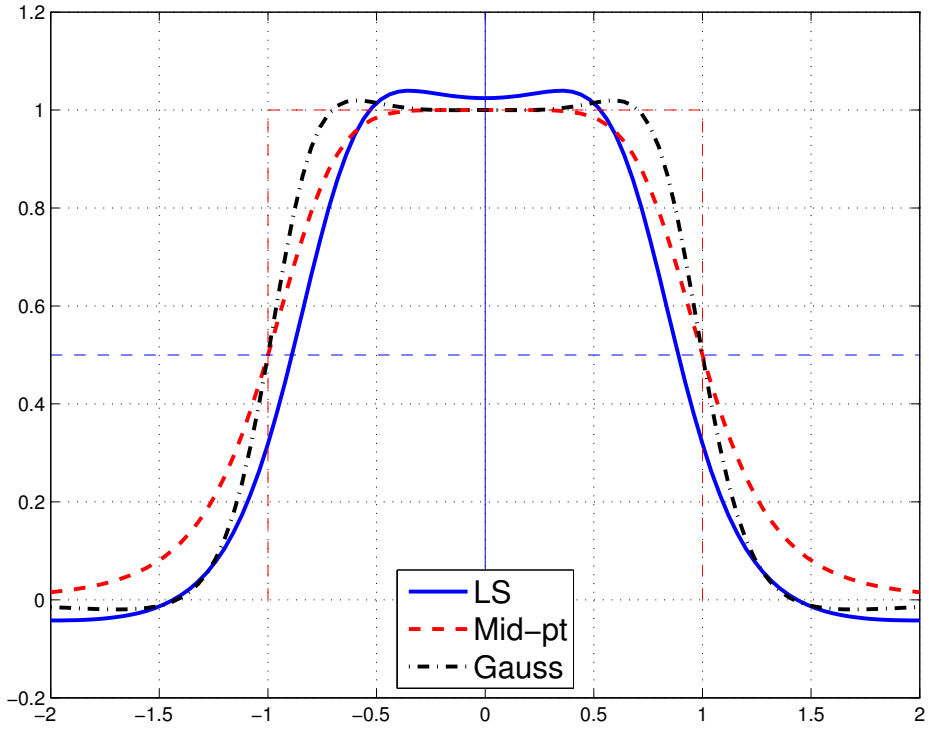
Better rational filters

➤ When using rational filters often one resorts to Cauchy integrals :

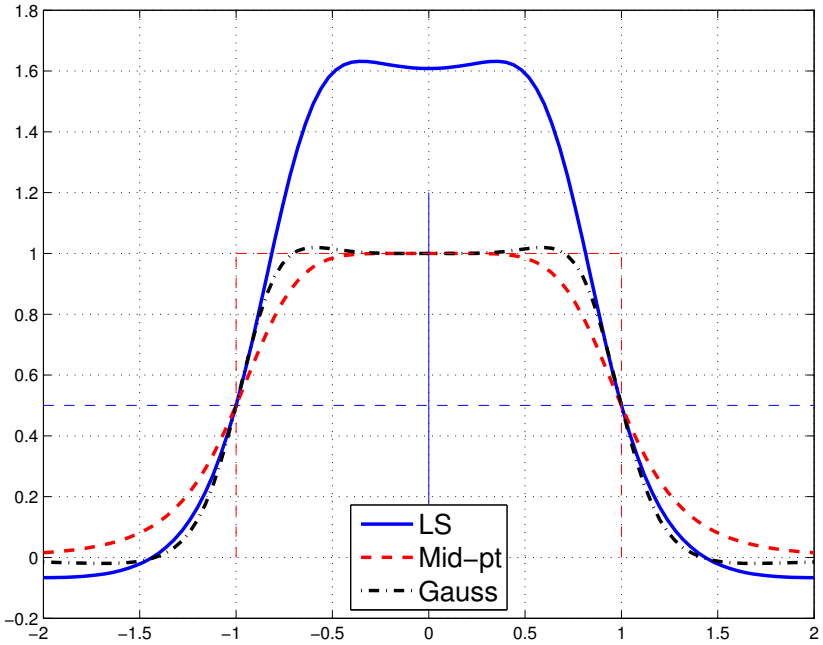
Spectral projector $\boldsymbol{P = \frac{-1}{2i\pi}\int_\Gamma (A - sI)^{-1} ds}$ + *Numer. Integ.*

➤ Approximation theory viewpoint:
Find rational function that approximates step function in $[-1, 1]$ *[after shifting + scaling]*

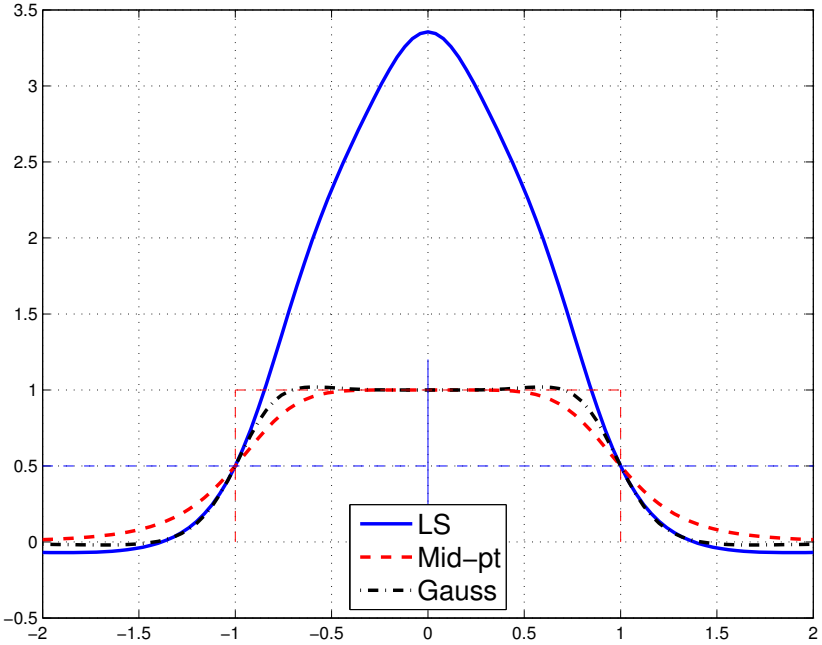
➤ e.g., work by S. Guettel et al. 2014. Uniform approx.



Different Look at the 3 curves

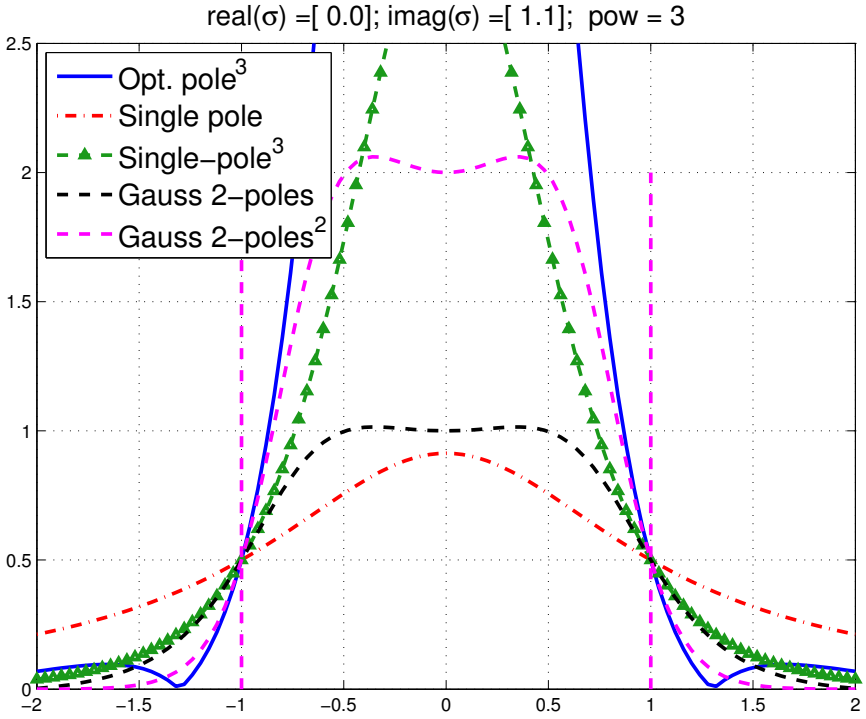


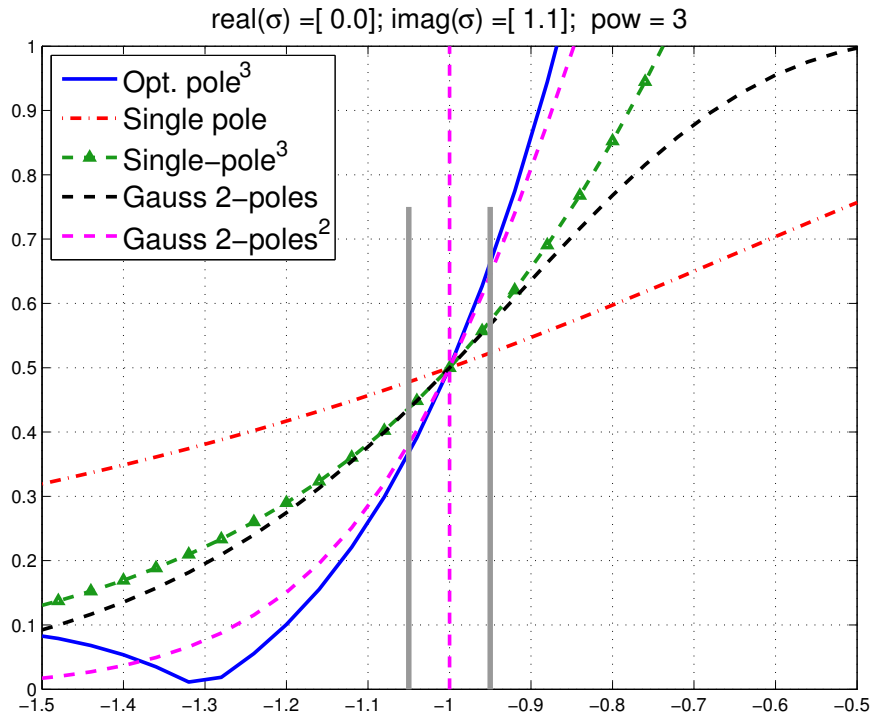
What about this case?



- The blue curve on the right is likely to give better results than the other 2 when subspace iteration is used.
- Want large values inside $[-1, 1]$ and small ones outside, but do not care much how well step function is approximated

What makes a good filter





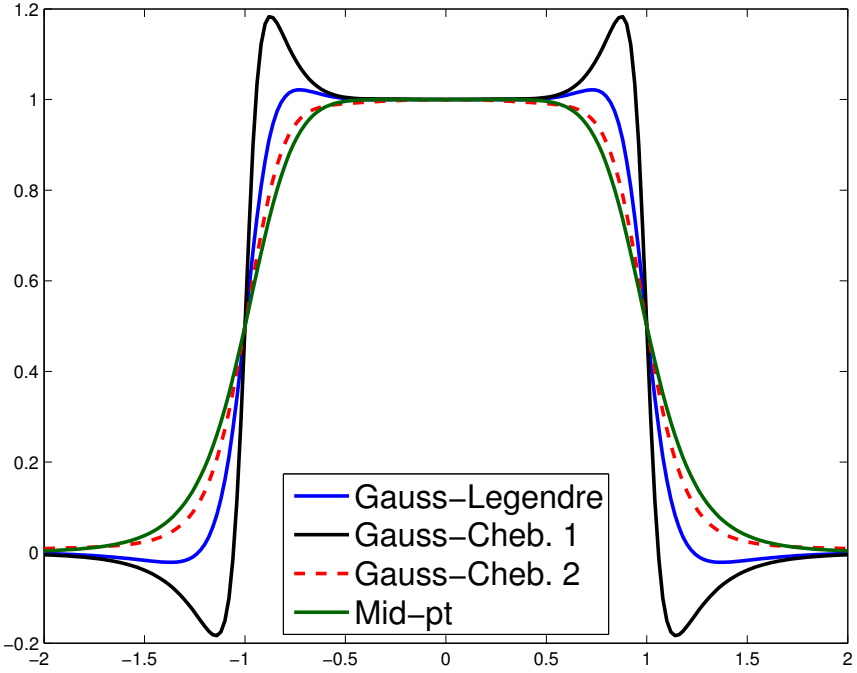
➤ Assume subspace iteration is used with above filters. Which filter will give better convergence?

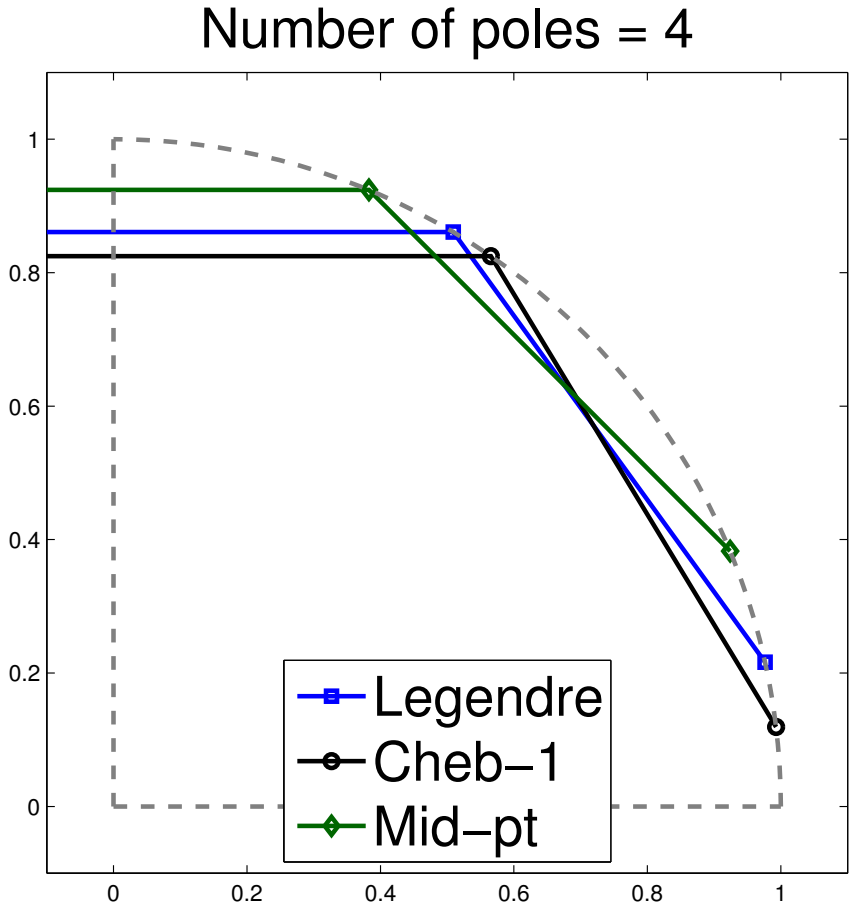
➤ Simplest and best indicator of performance of a filter is the magnitude of its derivative at -1 (or 1)

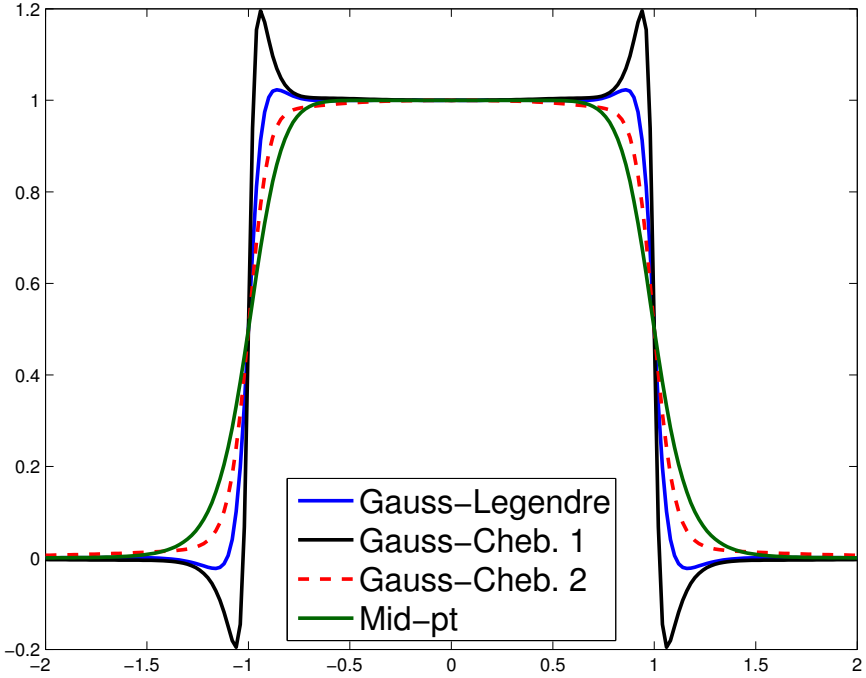
The Cauchy integral viewpoint

➤ Standard Mid-point, Gauss-Chebyshev (1st, 2nd) and Gauss-Legendre quadratures. Left: filters, right: poles

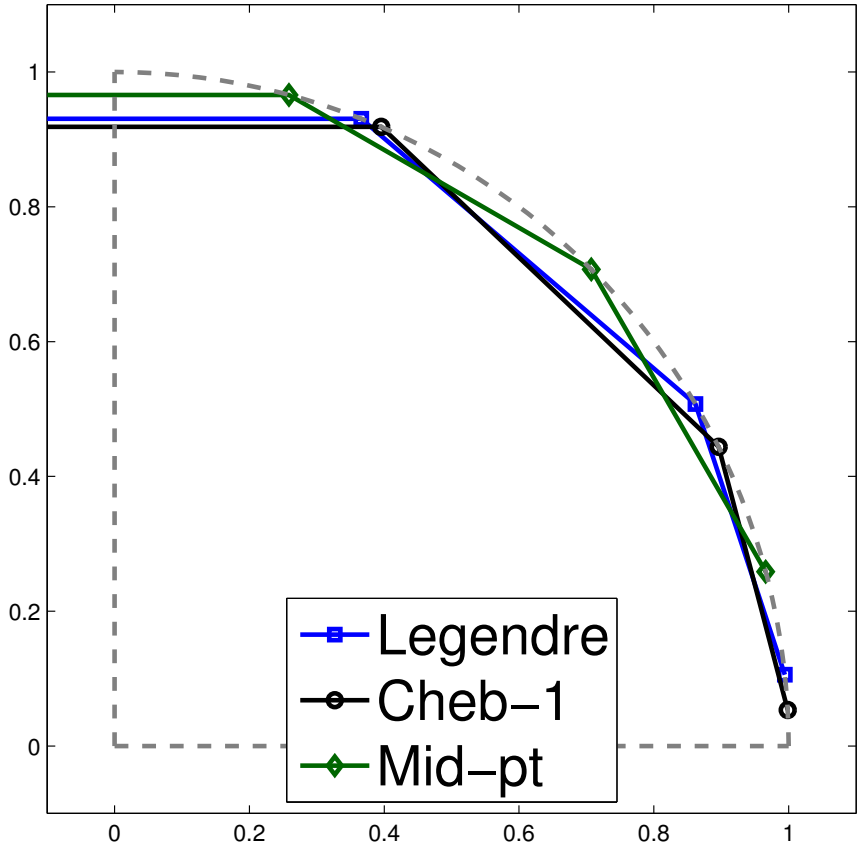
Scaling used so $\phi(-1) = \frac{1}{2}$







Number of poles = 6



- Notice how the sharper curves have poles close to real axis

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

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

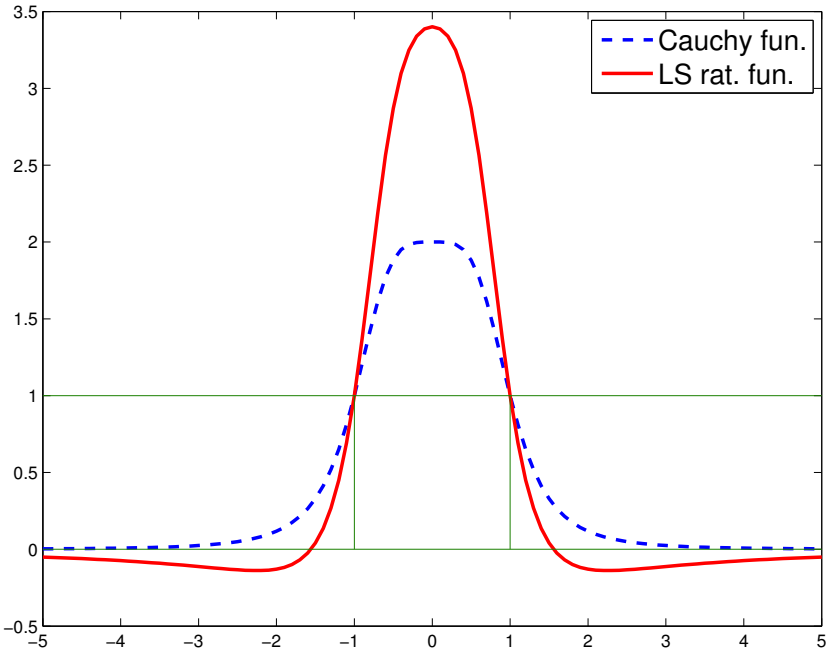
- $h(t)$ = step function $\chi_{[-1,1]}$.
- $w(t)$= weight function.

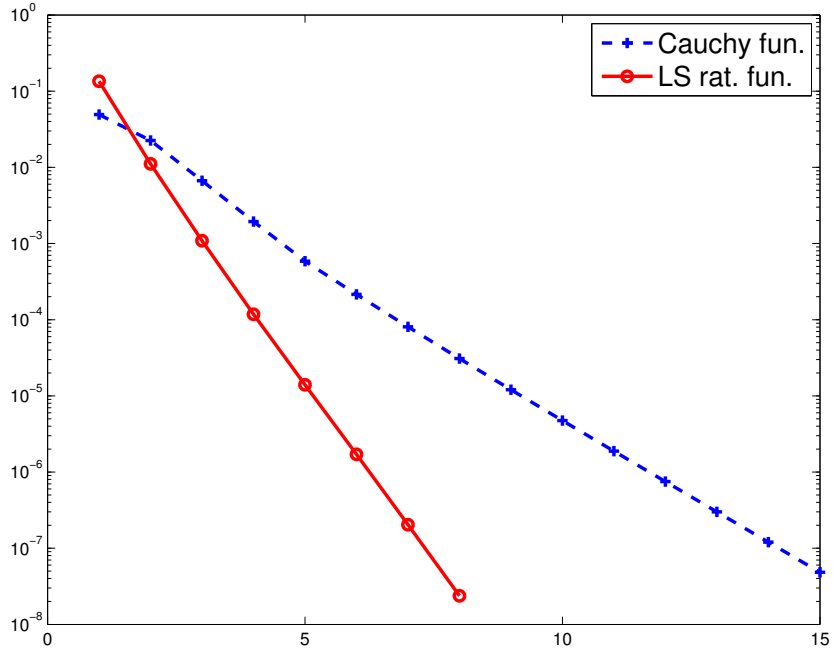
For example $a = 10$, $\beta = 0.1$

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

How does this work?

- A small example : Laplacean on a 43×53 grid. ($n = 2279$)
- Take 4 poles obtained from mid-point rule($N_c = 2$ on each 1/2 plane)
- Want: eigenvalues inside $[0,\ 0.2]$. There are $nev = 31$ of them.
- Use 1) standard subspace iteration + Cauchy (FEAST) then 2) subspace iteration + LS Rat. Appox.
- Use subspace of dim $nev + 6$
- $\beta = 0.2$



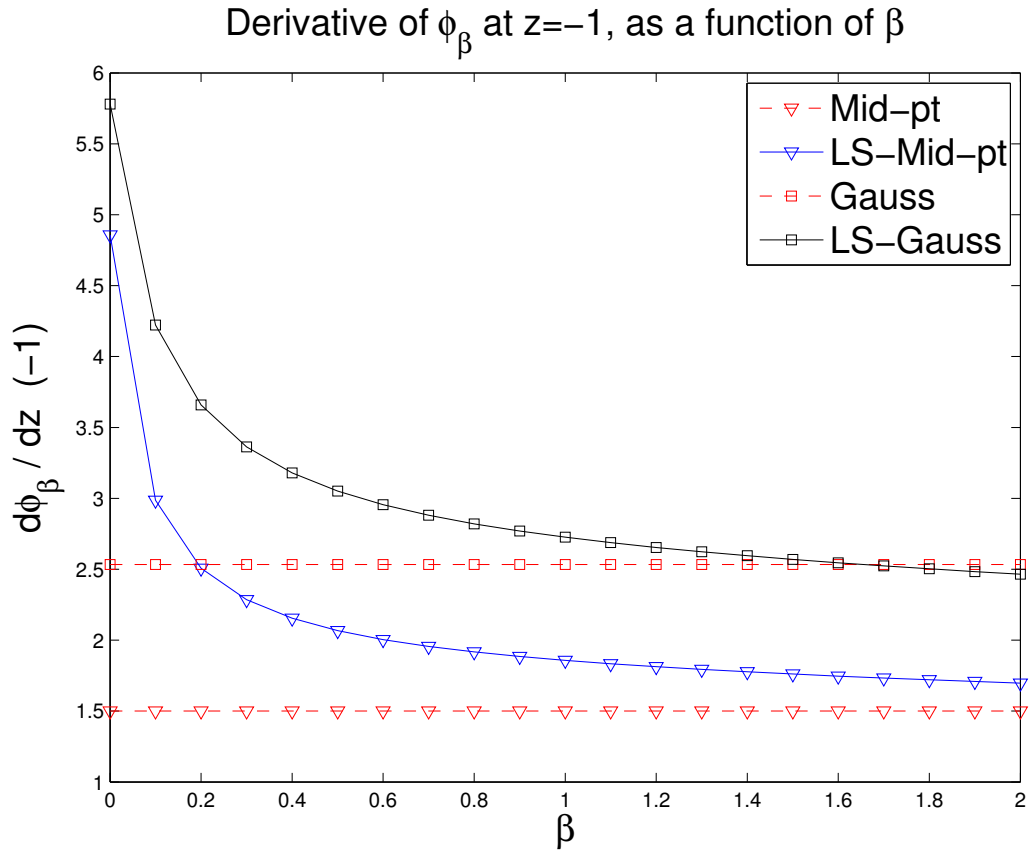


- LS Uses the same poles + same factorizations as Cauchy but
- ... much faster as expected from a look at the curves of the functions

- Other advantages:
  - Can select poles far away from real axis $\longrightarrow$ faster iterative solvers [E. Di Napoli, YS, et al-, work in progress]
  - Can use multiple poles (!)
  - Very flexible – can be adapted to many situations

Influence of parameter β

- Recall: large $\beta \rightarrow$ better approximation to h – not needed
- Smaller values are better



Better rational filters: Multiple poles

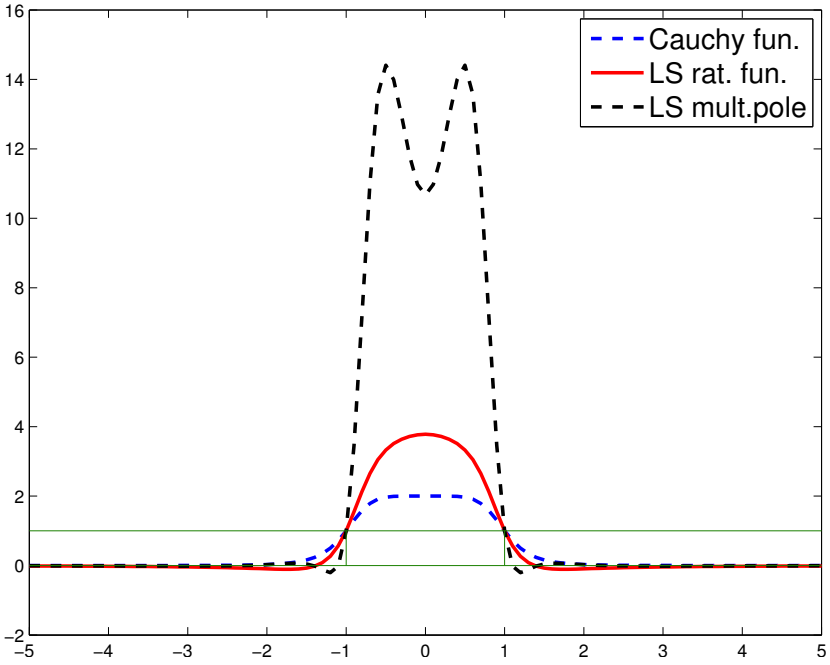
- Current choices: Mid-point/Trapezoidal rule, Gauss, Zolotarev,...
- None of these allows for repeated ('multiple') poles e.g., with one pole of multuplicity k:

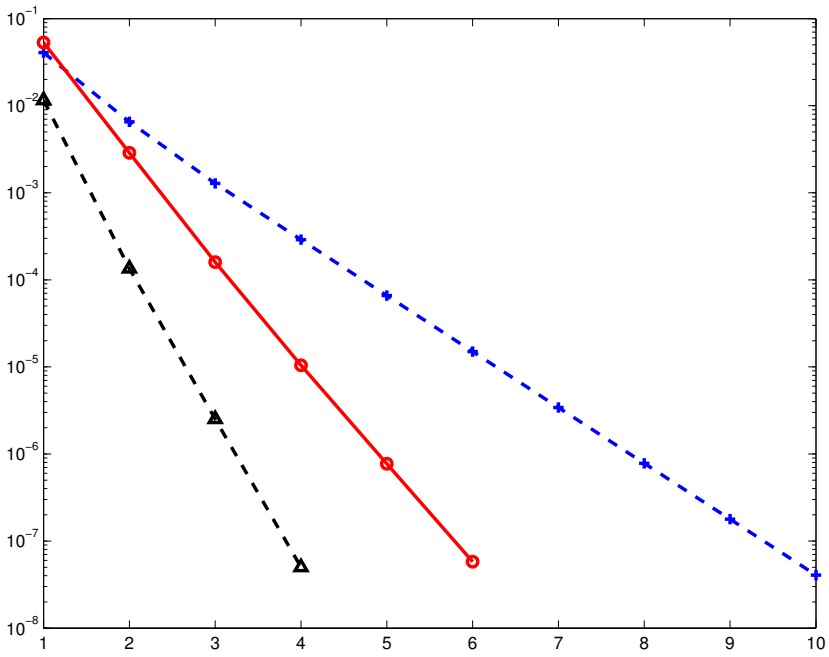
$$\phi(z) = \frac{\alpha_1}{z-\sigma} + \frac{\alpha_2}{(z-\sigma)^2} + \cdots + \frac{\alpha_k}{(z-\sigma)^k}$$

- Advantage: Fewer exact or incomplete factorizations needed for solves
- Next: Illustration with same example as before

Better rational filters: Example

- Take same example as before 43×53 Laplacean
- Now take 6 poles [3×2 midpoint rule]
- Repeat each pole [double poles.]





- General form

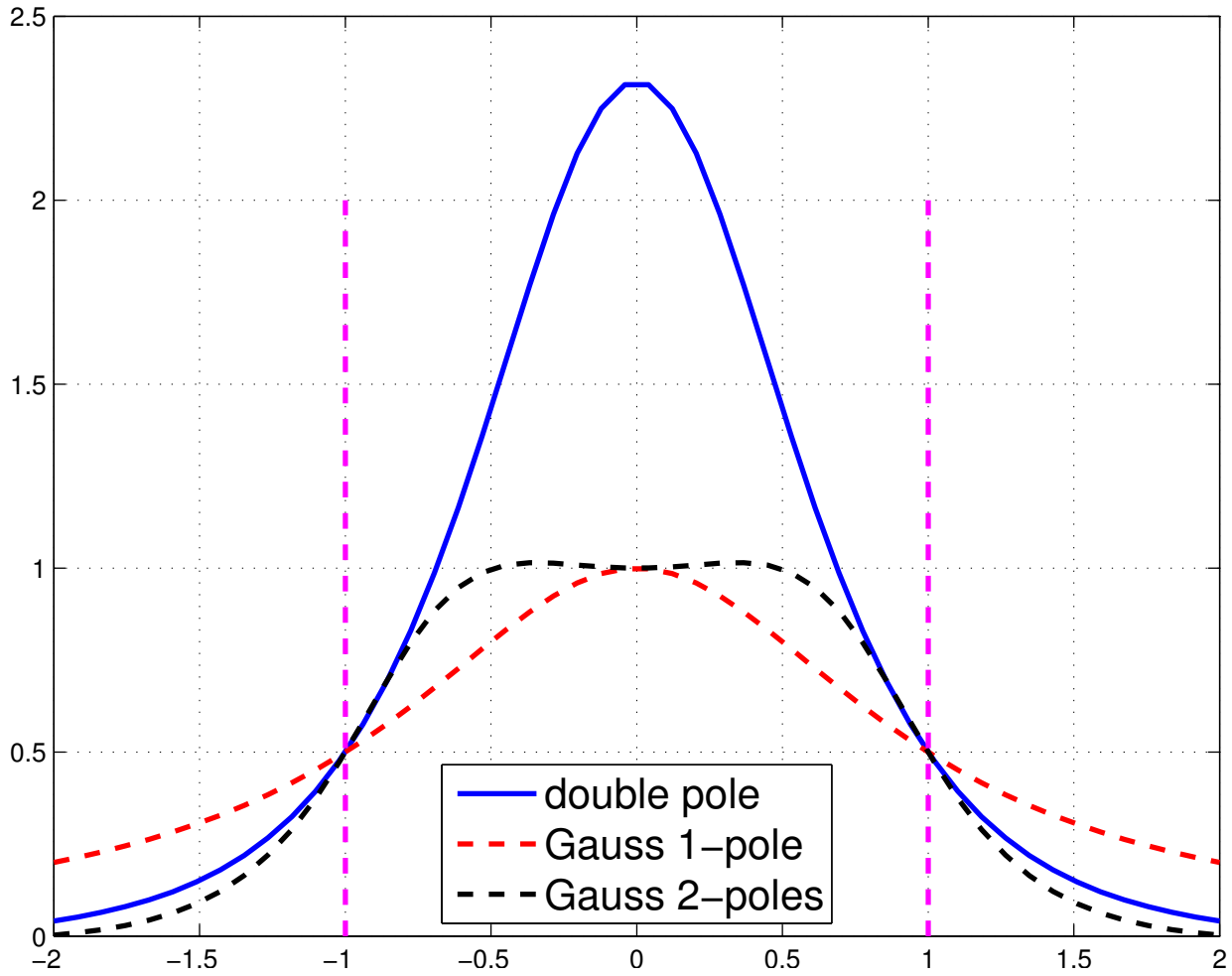
$$\phi(z) = \sum_{i=1}^{N_p} \sum_{j=1}^{k_i} \frac{\alpha_{ij}}{(z - z_i)^j}$$

- We then need to minimize (as before)

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

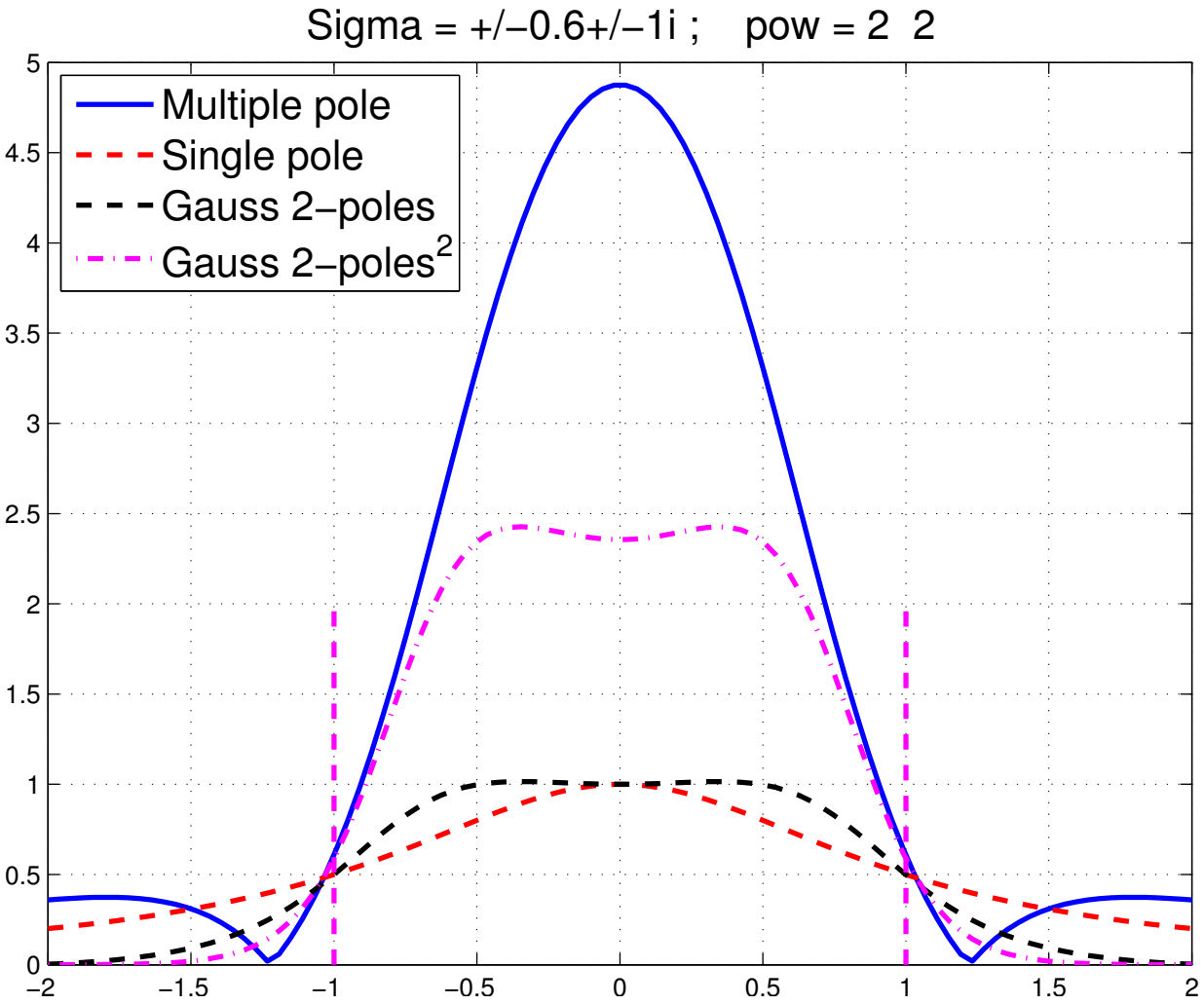
- Need to exploit partial fraction expansions
- Straightforward extension [but somewhat more cumbersome]

Next: See what we can do with *one* double pole



Who needs a circle?

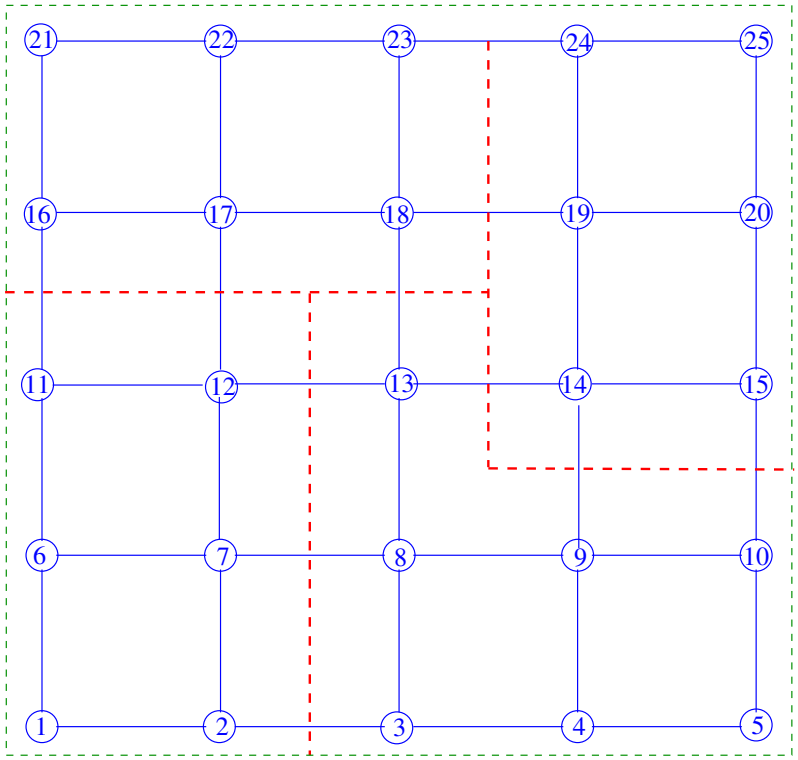
Two poles^2 + comparison with compounding



SPECTRAL SCHUR COMPLEMENT TECHNIQUES

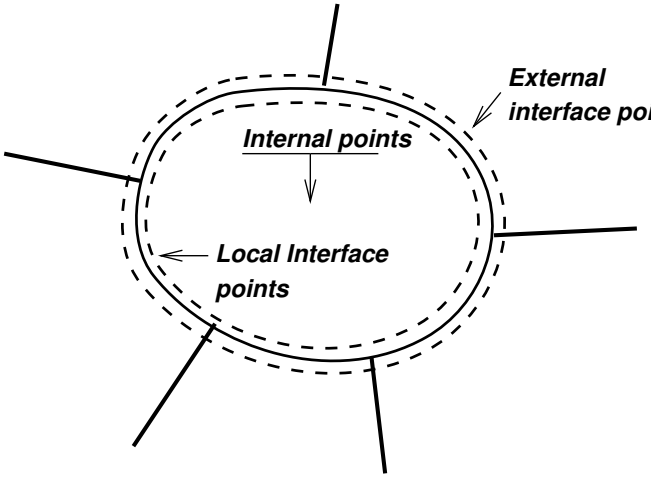
Introduction: Domain-Decomposition

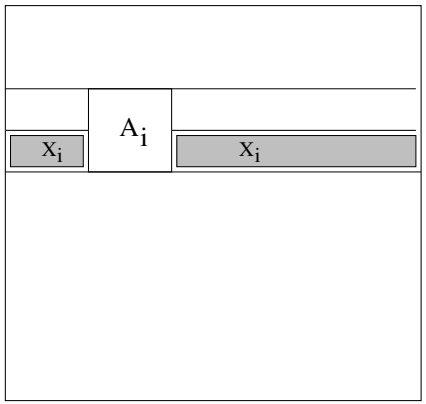
* Joint work with Vasilis Kalantzis and Ruipeng Li



➤ Partition graph using edge-separators ('vertex-based partitioning')

Distributed graph and its matrix representation





- Stack all interior variables $u_1, u_2, \cdots, u_p$ into a vector u, then interface variables y

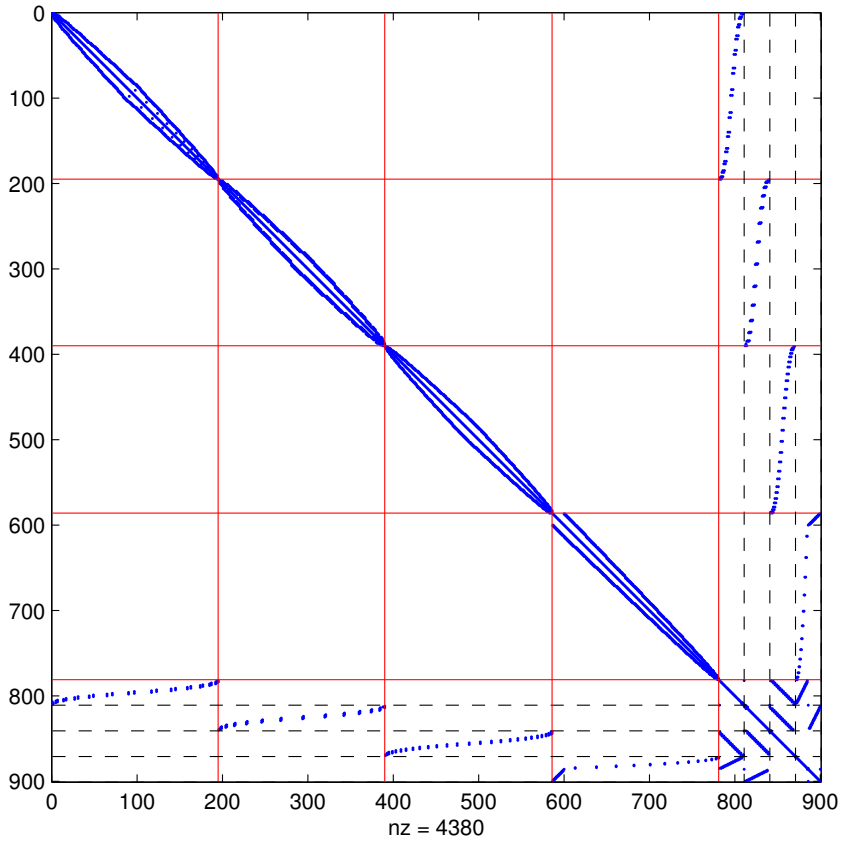
- Result:

$$\underbrace{\begin{pmatrix} B_1 & & & E_1 \\ & B_2 & & E_2 \\ \vdots & & \ddots & \vdots \\ & & B_p & E_p \\ E_1^T & E_2^T & \dots & E_p^T \quad C \end{pmatrix}}_{PAP^T} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_p \\ y \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_p \\ y \end{pmatrix}$$

Notation:

Write as:

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix}$$



The spectral Schur complement

- Eliminating the u_i's we get

$$\begin{pmatrix} S_1(\lambda) & E_{12} & \cdots & E_{1p} \\ E_{21} & S_2(\lambda) & \cdots & E_{2p} \\ \vdots & & \ddots & \vdots \\ E_{p1}^\top & E_{p2}^\top & \cdots & S_p(\lambda) \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} = 0$$

- $S_i(\lambda) = C_i - \lambda I - E_i^\top (B_i - \lambda I)^{-1} E_i$
- Interface problem (non-linear): $S(\lambda) y(\lambda) = 0.$
- Top part can be recovered as $u_i = -(B - \lambda I)^{-1} E_i y(\lambda)$.
- See also AMLS [Bennighof, Lehoucq, 2003]

Spectral Schur complement (cont.)

State problem as:

- Find $\sigma \in \mathbb{R}$ such that

One eigenvalue of $S(\sigma) \equiv 0$, or,

➤ $\mu(\sigma) = 0$ where $\mu(\sigma)$ == smallest ($|.|$) eig of $S(\sigma)$.

➤ Can treat $\mu(\sigma)$ as a function $\rightarrow$ root-finding problem.

➤ The function $\mu(\sigma)$ is analytic for any $\sigma \notin \Lambda(B)$ with

$$\frac{d\mu(\sigma)}{d\sigma} = -1 - \frac{\|(B - \sigma I)^{-1} E y(\sigma)\|_2^2}{\|y(\sigma)\|_2^2}.$$

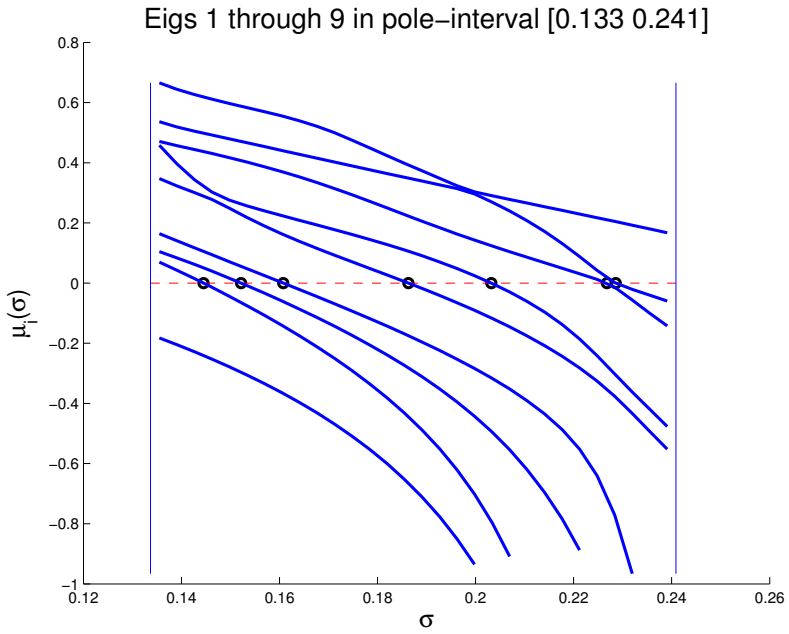
Basic algorithm - Newton's scheme

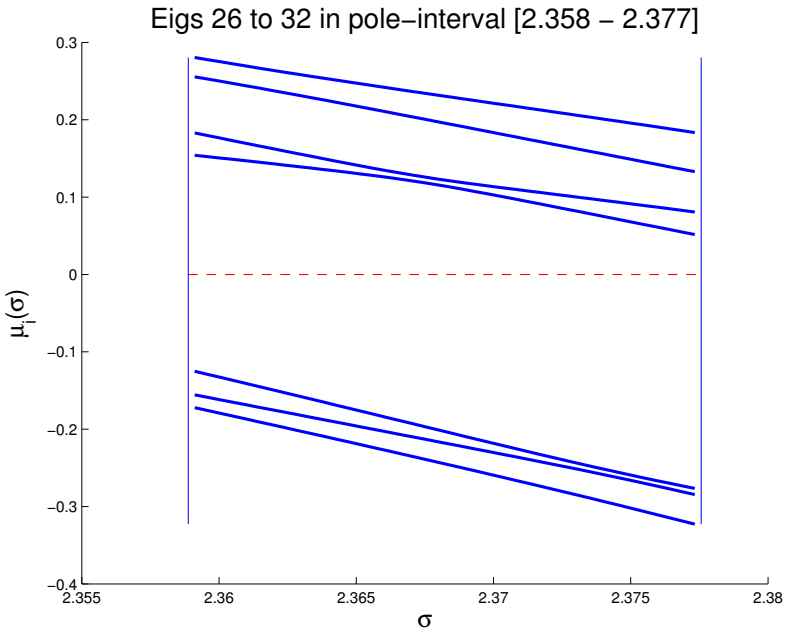
- We can formulate a Newton-based algorithm.

ALGORITHM : 1. *Newton Scheme*

1. *Select initial* σ
2. ***Repeat:***
3. *Compute* $\mu(\sigma) =$ *Smallest eigenvalue in modulus*
4. *of* $S(\sigma)$ *& associated eigenvector* $y(\sigma)$
5. *Set* $\eta := \|(B - \sigma I)^{-1} E y(\sigma)\|_2$
6. *Set* $\sigma := \sigma + \mu(\sigma)/(1 + \eta^2)$
7. ***Until:*** $|\mu(\sigma)| \leq \mathrm{tol}$

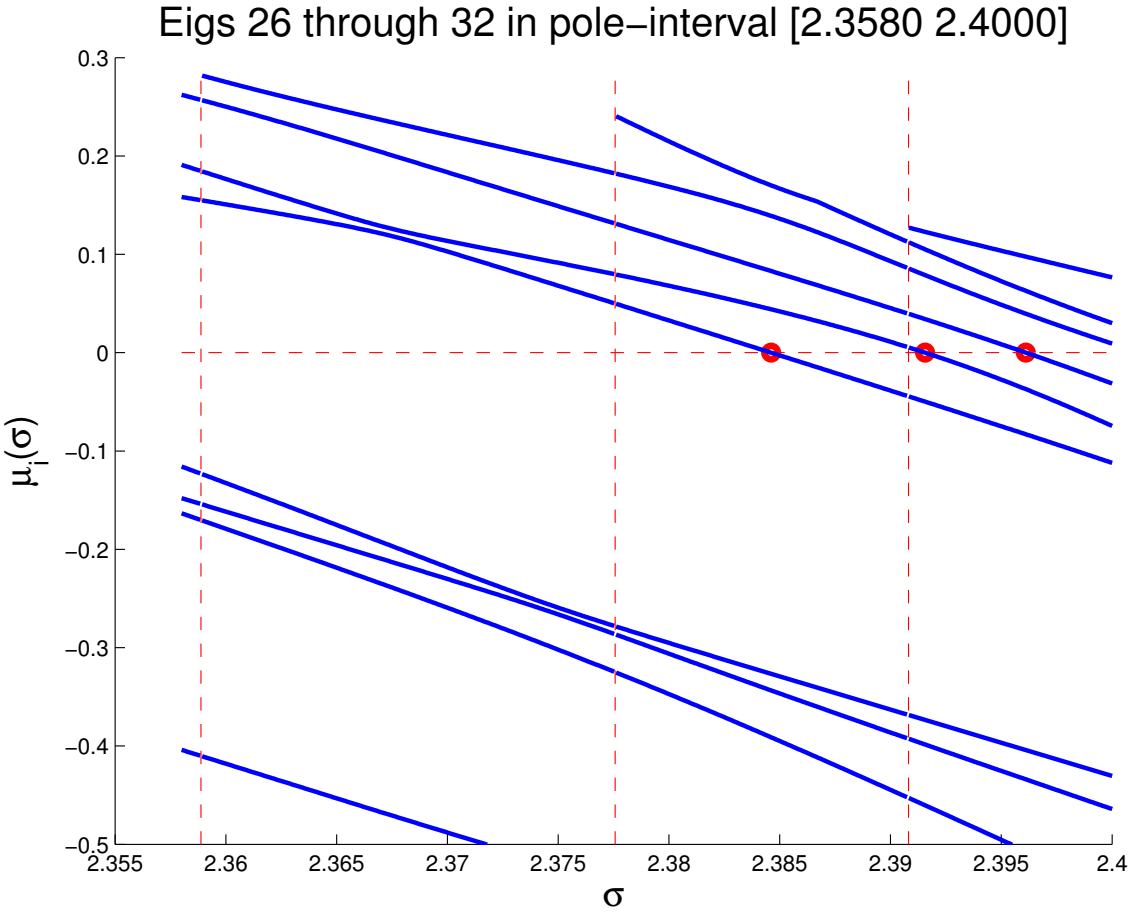
Short illustration - eigen-branches between two poles





➤ There may be a few, or no, eigenvalues λ between two poles.

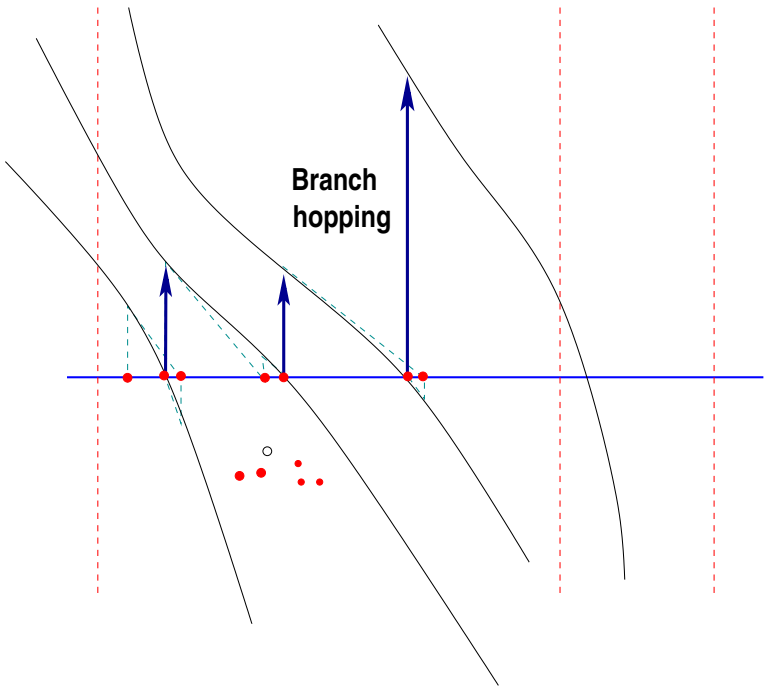
Eigen-branches across the poles

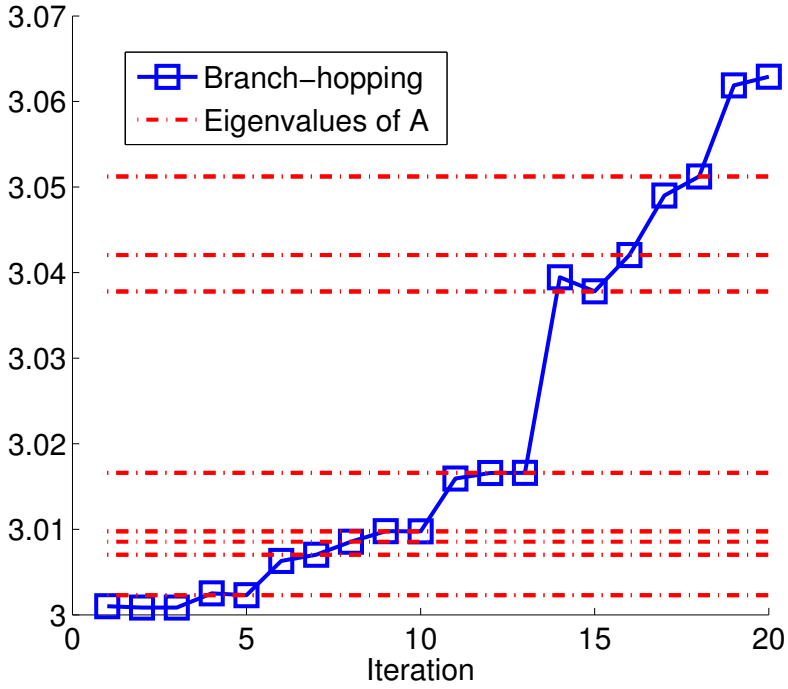


$$S(\sigma) = C - \sigma I - E^T(B - \sigma I)^{-1}E \equiv C - \sigma I - \sum_{i=1}^{m} \frac{w_i w_i^T}{\theta_i - \sigma}$$

Branch-hopping

- Once we converge ...
- ... start Newton from point on branch immediatly above current root.





Evaluating $\mu(\sigma)$

Inverse Iteration

- For any σ we just need one (two) eigenvalues of $S(\sigma)$.
- Good setting for "Inverse-Iteration" type approaches.

Lanczos algorithm

- Tends to be expensive for large p and eigenvalues deep inside spectrum

Numerical experiments

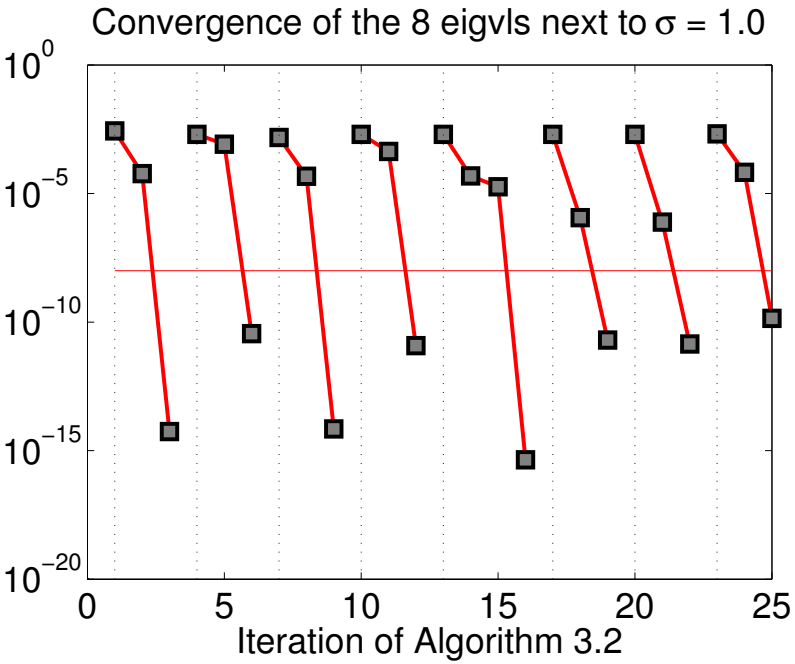
Some details

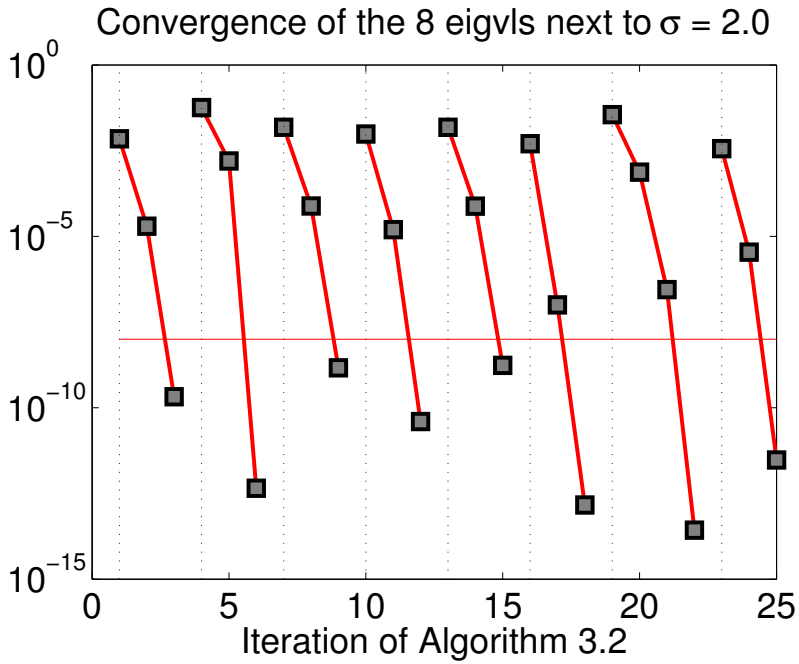
- Implementation in MPI-C++ using PETSc
- Tests performed on Itasca Linux cluster @ MSI.

The model problem

- Tests on 3-D dicretized Laplacians (7pt. st. – FD).
- We use n_x, n_y, n_z to denote the three dimensions.
- tol set to $1e-12$.
- Single-level partitioning – One node per sub-domain.

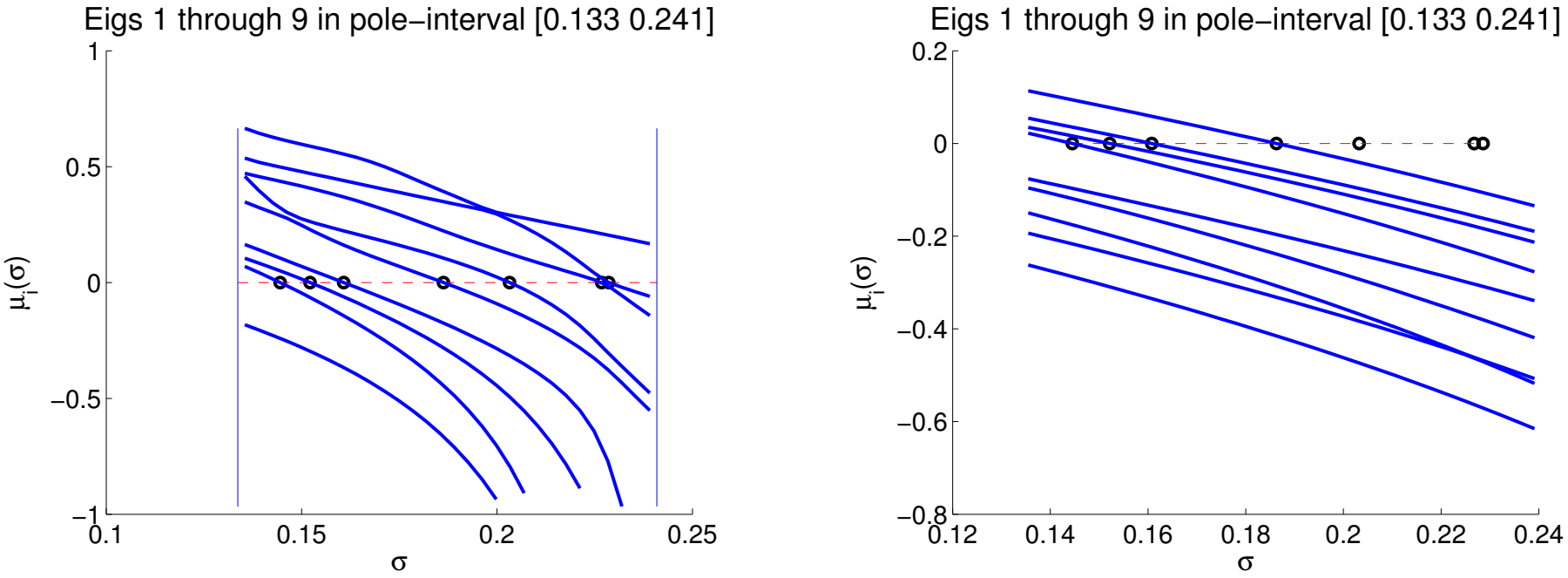
Example of convergence history





Rel. res. for a few consecutive eigenvalues.
Left $40 \times 40 \times 20$ grid. Right: $20 \times 20 \times 20$

Effect of number of domains p on convergence



Eigen-branches $\mu_1(\sigma), \ldots, \mu_9(\sigma)$ in $[0.133, 0.241]$ for a $33 \times 23 \times 1$ grid. Left: $p = 4$, right: $p = 16$.

Numerical experiments: Parallel tests

- Tests performed on Itasca Linux cluster @ MSI.
- Each node is a two-socket, quad-core 2.8 GHz Intel Xeon X5560 “Nehalem EP" with 24 GB of system memory.
- Interconnection : 40-gigabit QDR InfiniBand (IB).

The model problem

- Tests on 3-D dicretized Laplacians (7pt. st. – FD).
- We use n_x, n_y, n_z to denote the three dimensions.
- tol set to $1e-12$.

Wall-clock timings to compute the first $k = 1$ and $k = 5$ eigenpairs to the right of σ.

			$\sigma = 0.0$		$\sigma = 0.5$	
	(p,k)	s	Sec	It	Sec	It
$71 \times 70 \times 69$	(32,1)	65647	1.66	3	11.7	4
	(32,5)	— —	10.1	15	68.2	19
	(64,1)	83358	0.47	3	5.20	4
	(64,5)	— —	3.20	14	31.2	19
	(128,1)	108508	**0.16**	**3**	**1.90**	**4**
	(128,5)	— —	**1.10**	**14**	**11.7**	**18**
$101 \times 100 \times 99$	(64,1)	181901	5.90	3	41.1	3
	(64,5)	— —	28.3	15	221.5	15
	(128,1)	230849	1.18	3	7.80	3
	(128,5)	— —	6.24	15	41.5	14
	(256,1)	293626	**0.65**	**3**	**2.90**	**3**
	(256,5)	— —	**3.80**	**15**	**14.8**	**14**

	(p,k)	s	$\sigma = 0.0$ Sec	$\sigma = 0.0$ It	$\sigma = 0.5$ Sec	$\sigma = 0.5$ It
601×600	(16,1)	7951	0.65	3	3.10	3
	(16,5)	— —	4.42	15	15.9	15
	(32,1)	12377	0.26	3	2.90	3
	(32,5)	— —	1.60	14	16.4	15
	(64,1)	18495	**0.20**	**3**	**1.10**	**3**
	(64,5)	— —	**1.10**	**14**	**5.40**	**14**
801×800	(32,1)	16673	1.83	3	11.1	3
	(32,5)	— —	10.2	15	65.1	15
	(64,1)	24945	0.73	3	5.00	3
	(64,5)	— —	4.10	15	28.20	14
	(128,1)	36611	**0.31**	**3**	**2.10**	**3**
	(128,5)	— —	**1.80**	**15**	**9.70**	**14**

Conclusion

Part I: Polynomial filtering

- Polnym. Filter. appealing when # of eigenvectors to be computed is large and when Matvecs are inexpensive
- Will not work too well for generalized eigenvalue problem
- Will not work well for spectra with very large outliers.

Part II: Rational filtering

- We must rethink the way we view Rational filtering - away from Cauchy and into approximation of functions. LS approach is flexible, easy to implement, easy to understand.

Part III: Domain Decomposition

- We *must* combine DD with any filtering technique [rational or polynomial]
- Many ideas still to explore in Domain Decomposition for interior eigenvalue problems

- `Filtlan` code available here:

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