Prirodoslovno-matematički fakultet
Matematički odsjek
Sveučilište u Zagrebu

Hrvatska zaklada za znanost

Numerical resolvent calculus and filtered subspace iteration for self-adjoint operators

ConDys – Second project meeting,
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Joint work with Jay Goplakrishnan and Jeffrey Ovall

Outline

1. About the problem
2. About the method
3. Discretizing the resolvents
4. Numerical experiments

Model operator

$$\mathcal{A}u = -\triangle u - Vu, \qquad u \in H^1_*(\Omega).$$

- $\Omega \subset \mathbf{R}^d$ open and bounded
- $\mathcal{A}$ self-adjoint and unbounded
- $(\xi - \mathcal{A})^{-1}$ operator valued function
- $\mathrm{Spec}(\mathcal{A})$ is countable without finite accumulation points.
- Notation: $\mathcal{A}\psi_i = \lambda_i\psi_i$, and $-\|V\| \leq \lambda_1 \leq \lambda_2 \leq \cdots$
- We are counting eigenvalues with multiplicity.
- Variational (energy) scalar product $(u, v)_{\mathcal{V}} = \mathfrak{a}[u, v]$, $u, v \in H^1_*(\Omega)$.

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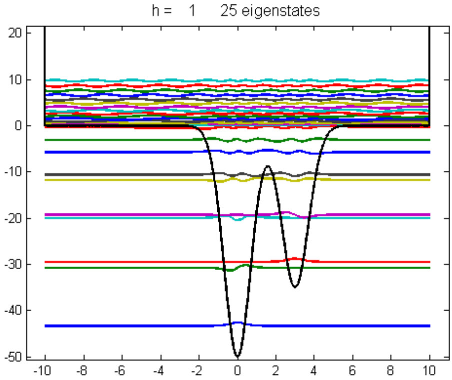
- $\mathcal{A}$ self-adjoint and unbounded
- $(\xi - \mathcal{A})^{-1}$ operator valued function
- It holds for the discrete spectrum $\mathrm{Spec}_{disc}(\mathcal{A}) \subset [\inf V, 0\rangle$
- Notation: $\mathcal{A}\psi_i = \lambda_i \psi_i$, and $-\|V\| \leq \lambda_1 \leq \lambda_2 \leq \cdots < 0$ are only isolated eigenvalues $\Rightarrow$ call them Λ
- We are counting eigenvalues with multiplicity.
- Variational (energy) scalar product $(u, v)_{\mathcal{V}} = \mathfrak{a}[u, v]$, $u, v \in H^1_*(\Omega)$.

Bounded and extended states

Quantum states from `chebfun` $V(t) = -50\left[\exp(-t^2) + 0.7\exp(-(t-3)^2)\right]$



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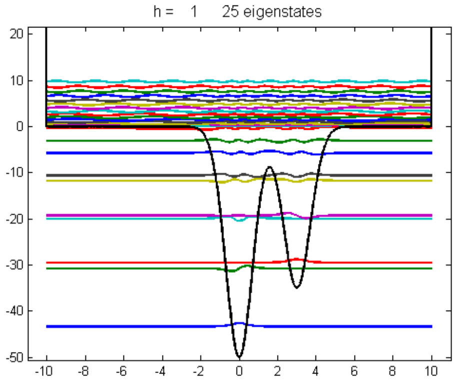

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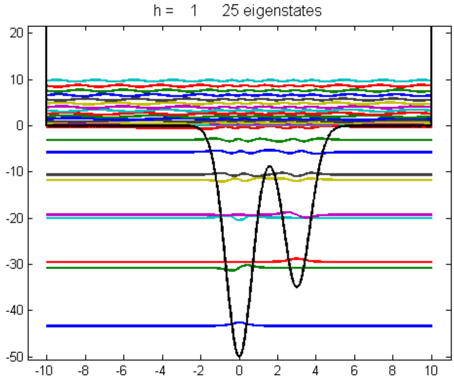
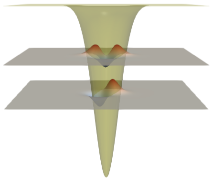
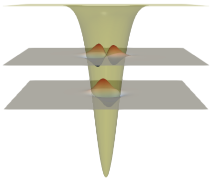
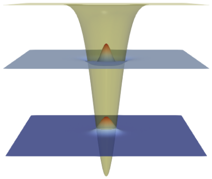


- We consider $\mathcal{A}_R$ on finite Ω_R.
- Perturbation argument: put a contour on $[-\|V\|, 0\rangle$, unwanted clustered eigenvalues in $[0, \infty\rangle$.

Bounded and extended states – also in 2D







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1. Start from sa self adjoint operator A and its spectrum $\Sigma(A)$
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3. Also, let E be the (m-dimensional) span of the corresponding eigenvectors,
4. And so the heroes are:

$$\Lambda = \{\lambda_1, \dots, \lambda_m\}, \qquad E = \mathrm{span}\{e_1, \dots, e_m\}, \qquad Ae_i = \lambda_i e_i.$$

The tools

- Let Γ be a simple closed contour enclosing Λ
- Define

$$r(z) = \frac{1}{2\pi\,1\mathbf{i}} \int_\Gamma (\xi - z)^{-1} = \begin{cases} 1 & , z \in G \\ 0 & , z \in \mathbb{C} \setminus (\Lambda \cup \Gamma) \end{cases}$$

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- $r_N(\cdot)$ is “ripping” Λ from $\Sigma(A)$!

Numerical analyst's take

- Rational approximation of r:

$$r(\xi) = \frac{1}{2\pi\,1\mathbf{i}} \int_\Gamma (\xi - z)^{-1} \; d\xi \approx r_N(\xi) = \sum_{i=1}^{N-1} \omega_i (z_i - \xi)^{-1} \; .$$

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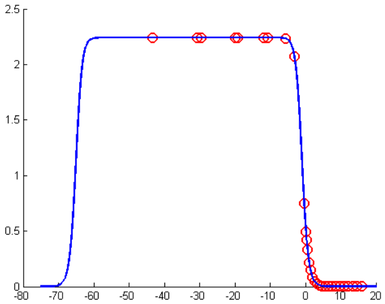
Note!

- The spectrum of $r_N(A)$ looks like



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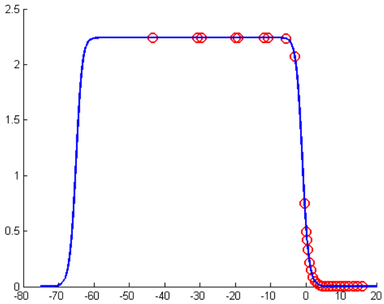


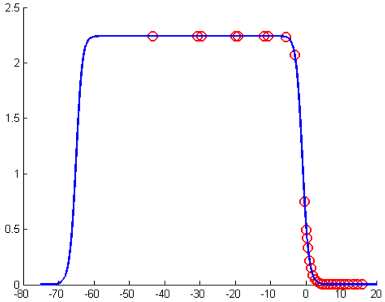
- Ideal for subspace iteration towards the dominant spectral component
- We know which singular values of $r_N(A)$ are big and which are small

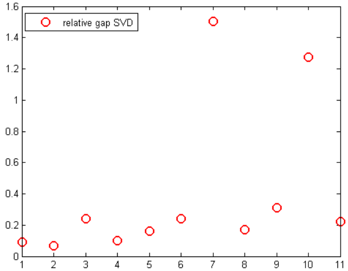
Spectral separation

That is – just by looking at properties of a priori known $r_N(\cdot)$ –

1. one can transform E into the dominant eigenspace of of the filtered operator $r_N(A)$ *provided* Λ separated from the unwanted component
2. we quantify the separation using $y \in \mathbb{R}$, $\delta > 0$ and $\gamma > 0$ such that $\Lambda \subset \{x \in \mathbb{R} : |x - y| < \gamma\}, \qquad \Sigma(A) \backslash \Lambda \subset \{x \in \mathbb{R} : |x - y| \geq (1 + \delta)\gamma\}$
3. we detect separation form the decay rates of the singular values of $r_N(A)$

Spectral separation SVD picture





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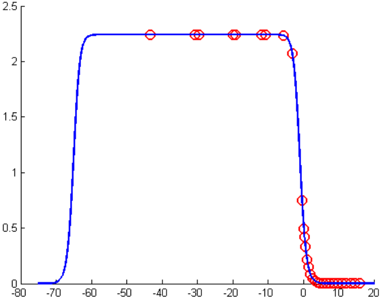
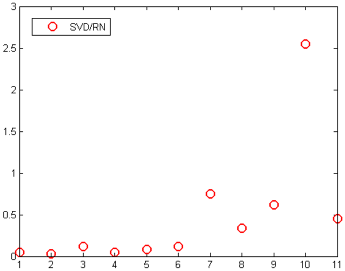
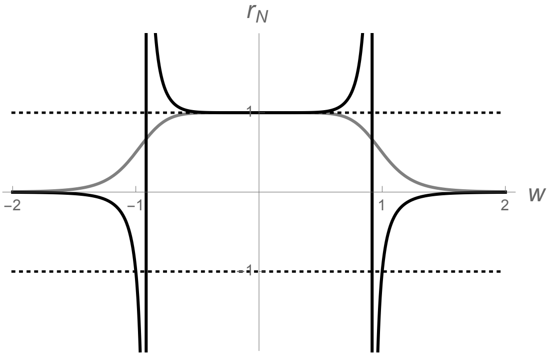
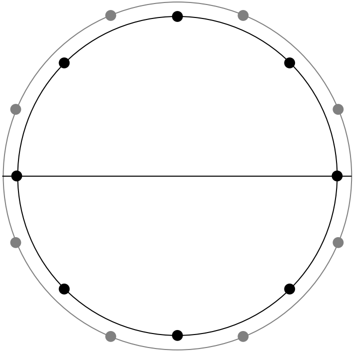




Study circle filters





The ratio

$$\kappa = \sup_{\mu \in \Sigma(A) \setminus \Lambda} |r_N(\mu)| / \min_{\lambda \in \Lambda} |r_N(\lambda)| \tag{1}$$

is a measure of filter quality (for separating spectral components).

Let y, γ, be as before, then

$$W = \sum_{k=0}^{N-1} |w_k|, \qquad \hat{\kappa} = \frac{\sup_{x \in O_{\delta,\gamma}^y} |r_N(x)|}{\inf_{x \in I_\gamma^y} |r_N(x)|}\,, \tag{2}$$

where $O_{\delta,\gamma}^y = \{x \in \mathbb{R} : |x - y| \geq (1+\delta)\gamma\}$ and $I_\gamma^y = \{x \in \mathbb{R} : |x - y| \leq \gamma\}$.

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where $O^y_{\delta,\gamma} = \{x \in \mathbb{R} : |x-y| \geq (1+\delta)\gamma\}$ and $I^y_\gamma = \{x \in \mathbb{R} : |x-y| \leq \gamma\}$.
Since $\kappa \leq \hat{\kappa}$, the quantity $\hat{\kappa}$ gives a bound for the filter quality.

Circle filters

Lemma (Properties of circle filters)

Consider the circle filters givenon the previous figure. We have

$$W = \eta \leq \gamma, \qquad \textit{for both filters.} \tag{3a}$$

If N is even, then

$$\hat{\kappa} = \frac{2}{(1+\delta)^N + 1} < 1 \qquad \textit{for the first filter,} \tag{3b}$$

$$\hat{\kappa} = \frac{1}{2(1+\delta)^N - 1} < 1 \qquad \textit{for the second filter.} \tag{3c}$$

γ *is* *radius*, δ *is the* *suck-in* *parameter.*

Separation assumption revisited

- How do we check the separation assumption
- By sampling

1. Apply S_N to a randomly selected orthonormal basis $\{u_1, \cdots, u_b\}$
2. Numerically determine the dimension using SVD.
3. Rapid decay of singular values indicates right dimension. Small for the circle filter (properties of the known rational function)means much smaller than $1/2$!
4. It is an unbiased estimator of the number of eigenvalues inside the circle.

FEAST = filtered subspace iteration + RR extraction

- Let $\mathcal{W}$ be a (complex) Hilbert space and let $B : \mathcal{W} \to \mathcal{W}$ be a bounded linear operator.
- Let Υ be a finite set of eigenvalues of finite multiplicity of B that are isolated from the rest of $\Sigma(B)$.
- Consider $\tilde{B}_\ell = B + \Delta_\ell$ where $\Delta_\ell : \mathcal{W} \to \mathcal{W}$ is a bounded linear operator representing perturbations at step l of the iteration.
- The iterations are started using a given initial finite-dimensional subspace $Q_0 \subset \mathcal{W}$.
- At step ℓ, the *inexact subspace iteration* computes the subspace

$$Q_\ell = \tilde{B}_\ell Q_{\ell-1}, \qquad \ell = 1, 2, \ldots. \tag{4}$$

FEAST = filtered subspace iteration + RR extraction

Lemma

Suppose $\dim(PQ_0) = \dim(Ran(P))$*. Then for each* $0 \neq \mu \in \Upsilon$ *and* $0 \neq v \in \mathcal{W}$ *satisfying* $Bv = \mu v$*, there is a sequence* $q^{(\ell)}$*,* $\ell = 0, 1, 2, \ldots,$ *such that* $q^{(\ell)} \in Q_\ell$ *and*

$$v - q^{(\ell)} = \frac{1}{\mu^\ell} B^\ell (I - P)(v - q^{(0)}) + \frac{1}{\mu^\ell} \left[B^\ell - \left(\tilde{B}_\ell \tilde{B}_{\ell-1} \cdots \tilde{B}_1 \right) \right] q^{(0)}.$$

Ideal FEAST

- Set $\mu^* = \mathrm{rad}(B(I-P))$, the spectral radius of $B(I-P)$ in $\mathcal{W}$.
- The set Υ is a set of dominant eigenvalues if $\mu^* < |\mu|$ for all $\mu \in \Upsilon$.

Lemma

Suppose v and $q^{(\ell)}$ are as before, and $\Delta_\ell = 0$ for all ℓ. Then for any $\varepsilon > 0$, there is an integer $\ell_0 \geq 1$ such that for all $\ell \geq \ell_0$,

$$\|v - q^{(\ell)}\|_{\mathcal{W}} \leq \left|\frac{\varepsilon + \mu^*}{\mu}\right|^{\ell} \|v - q^{(0)}\|_{\mathcal{W}}.$$

If in addition B is selfadjoint with respect to the inner product of $\mathcal{W}$, then we may choose $\varepsilon = \ell_0 = 0$.

Assumptions

1. Consider the subspace iteration with perturbed filter $\tilde{B}^{(\ell)}$ set to $\tilde{S}_N^{(\ell)} = S_N + \Delta_\ell$
2. The perturbation size is measured by

$$\tilde{S}_N^{(\ell)} = S_N + \Delta_\ell, \qquad \|\Delta_\ell\|_{\mathcal{V}} \leq \tau \|S_N\|_{\mathcal{V}}. \tag{5}$$

Inexact subspace iteration – use a priori bounds on r_N!

$$r_N^* = \sup_{\lambda \in \Sigma(A) \setminus \Lambda} |r_N(\lambda)|, \qquad \kappa_i = \frac{r_N^*}{|r_N(\lambda_i)|}, \qquad \beta_i = \frac{\max_{1 \le j \le m} |r_N(\lambda_j)|}{|r_N(\lambda_i)|}. \tag{6}$$

Theorem

Let Q_ℓ be given by subspace iteration with $\tilde{B}_\ell = \tilde{S}_N^{(\ell)}$ starting from a $Q_0 \subseteq \mathcal{V}$ satisfying $\dim(SQ_0) = m$. Then for each e_i, there is a sequence $q_i^{(\ell)}$ in Q_ℓ satisfying

$$\|e_i - q_i^{(\ell)}\|_{\mathcal{V}} \le \kappa_i^\ell \|e_i - q_i^{(0)}\|_{\mathcal{V}} + [(1+\tau)^\ell - 1]\beta_i^\ell \|q_i^{(0)}\|_{\mathcal{V}}$$

for all $\ell \ge 0$ and $i = 1, \ldots, m$.

FEAST = filtered subspace iteration + RR extraction

Draws from two backgrounds!

- Contour integration
- Discrete resolvent approximation

FEAST = filtered subspace iteration + RR extraction

Eigenvalue Solvers Motivated by Contour Integrals:

- Sakurai, Sugiura. A projection method for generalized eigenvalue problems using numerical integration. J. Com. Math. Appl. (2003)
- Sakuria, Tadano. CIRR: A Rayleigh-Ritz type method with contour integral for generalized eigenvalue problems. Hok. Math. J. (2007)
- Polizzi. Density-matrix-based algorithm for solving eigenvalue problems. Phys. Rev. B (2009)
- Güttel, Polizzi, Tang, Viaud. Zolotarev quadrature rules and load balancing for the FEAST eigensolver. SIAM J. Sci. Comput. (2015)

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The perturbation: Discontinuos Petrov-Galerkin (DPG) projection

- Demkowicz, Gopalakrishnan. A primal DPG method without a first order reformulation. Comput. Math. Appl. (2013)
- Goplalkrishnan, Qui. An analysis of the practical DPG method. Math. Comput. (2014)

Outline

Rational approx. + FEM projection

- Rational approximation of r:

$$r(\xi) = \frac{1}{2\pi \, 1\mathbf{i}} \int_\Gamma (\xi - z)^{-1} \, d\xi \approx r_N(\xi) = \sum_{i=1}^{N-1} \omega_i (z_i - \xi)^{-1} \, .$$

- Take $R_h(z) : L^2(\Omega) \to \mathcal{V}_h$, and define

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- $R_h(.)$ is a FEM realization of the resolvent.

DPG resolvent approximations

Theorem

Suppose z lies in a bounded set of diameter D in the complex plane. There is a $C > 0$ depending only on D and the shape regularity of the mesh Ω_h such that for all $f \in L^2(\Omega)$,

$$\|R(z)f - R_h(z)f\|_{\mathcal{V}} \leq \frac{C}{d(z)} \left[\inf_{w_h \in L_h} \|u - w_h\|_{H^1(\Omega)} + \inf_{q_h \in RT_h} \|q - q_h\|_{H(\mathrm{div},\Omega)} \right]$$

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- For circle filter $\|S_N\|_{\mathcal{V}} > 1/2$ and so $\tau \leq \dfrac{2CW}{\min\limits_{k=1,\dots,N} d(z_k)^2} h_\ell^{\min(p,s_E)}$.

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- Can incorporate errors in iterative solvers or other linear algebra errors in computing the action of $R_h(z)$.

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- $u_{h,DPG} = \text{arg-min}_{x \in L_h} \|(z - A)x - f\|_{DG,-1}$

$\| \cdot \|_{DG,-1}$ is the discontinuous Galerkin approximation of $\| \cdot \|_{-1}$.

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$\|\cdot\|_{DG,-1}$ is the discontinuous Galerkin approximation of $\|\cdot\|_{-1}$.
Good theoretical framework because inf-sup is implicitly established.

Resolvent estimate

In a stronger norm under the assumption that there is a number s_E such that

$$\|u^f\|_{H^{1+s_E}(\Omega)} \leq C_{reg}\|f\|_{\mathcal{V}} \quad \text{for any } f \in E, \tag{7}$$

where u^f is such that $-\triangle u^f = f$, we get

$$\|R(z)v - R_h(z)v\|_{H^1(\Omega)} \leq \frac{C}{d(z)^2} h^{\min(p,s_E)} \|v\|_{H^1(\Omega)} \quad \text{for all } v \in E \tag{8}$$

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$$\|u^f\|_{H^{1+s_E}(\Omega)} \leq C_{reg}\|f\|_{\mathcal{V}} \quad \text{for any } f \in E, \tag{7}$$

where u^f is such that $-\triangle u^f = f$, we get

$$\|R(z)v - R_h(z)v\|_{H^1(\Omega)} \leq \frac{C}{d(z)^2} h^{\min(p,s_E)} \|v\|_{H^1(\Omega)} \quad \text{for all } v \in E \tag{8}$$

➡ Here we assumed that V_h is a piecewise polynomial space with polynomials of degree p.

All together

Based on

$$\|S_N - S_N^h\|_{\mathcal{V}} \leq W \max_{k=1,\dots,N} \|R_h(z_k) - R(z_k)\|_{\mathcal{V}} \to 0 \tag{9}$$

the estimates

All together

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the estimates

- for eigenvectors

$$\operatorname{gap}_{\mathcal{V}}(E, E_h) \leq C_N W \max_{k=1,\dots,N} \left\| \left(R(z_k) - R_h(z_k)\right)\big|_E \right\|_{\mathcal{V}}, \tag{10}$$

All together

Based on

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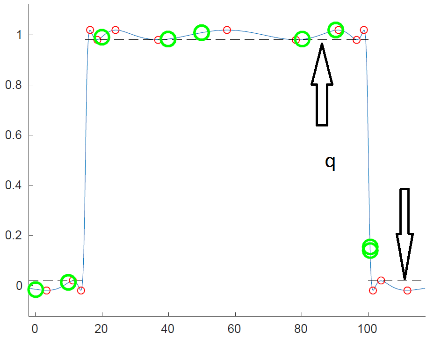
- and eigenvalues

$$\mathrm{dist}(\Lambda, \Lambda_h) \leq C_a \, \mathrm{gap}_{\mathcal{V}}(E, E_h)^2.$$

follow

Outline

The filter – a priori properties cf. S. Guettel



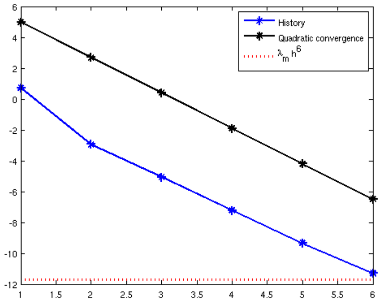
For MATLAB's users obligatory L-shape reference

h	λ_1 ERR	λ_1 NOC	λ_2 ERR	λ_2 NOC	λ_3 ERR	λ_3 NOC
2^{-2}	4.85e-02	——	1.34e-02	——	2.36e-02	——
2^{-3}	2.01e-02	1.27	2.18e-03	2.61	3.76e-03	2.65
2^{-4}	7.74e-03	1.37	1.97e-04	3.47	2.36e-04	3.99
2^{-5}	3.05e-03	1.34	2.18e-05	3.17	1.48e-05	3.99
2^{-6}	1.21e-03	1.34	2.81e-06	2.96	9.27e-07	4.00

Table: Eigenvalue errors (ERR) and numerical order of convergence (NOC) for the smallest three eigenvalues on the L-shaped domain.

pyeigfeast

A python implementation of FEAST + `ngsolve` realization of DPG.



pyeigfeast – Pythonic FEAST available on github

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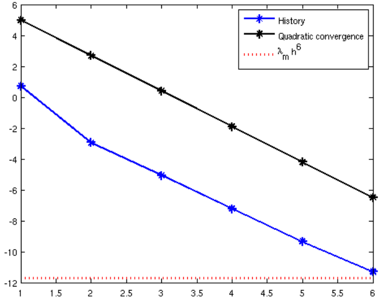

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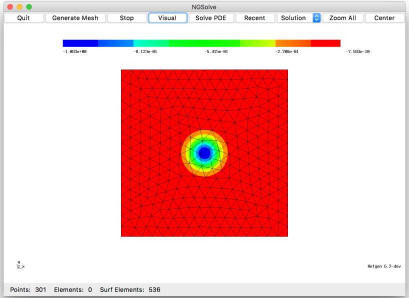

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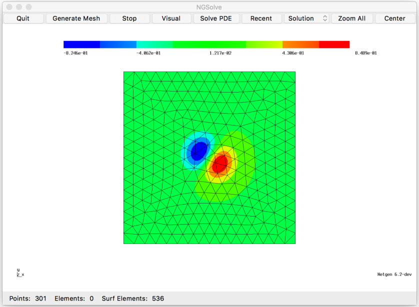

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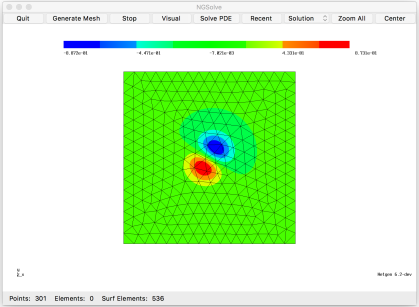

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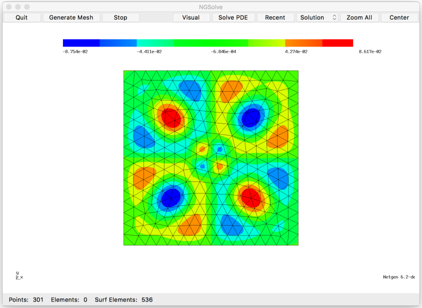
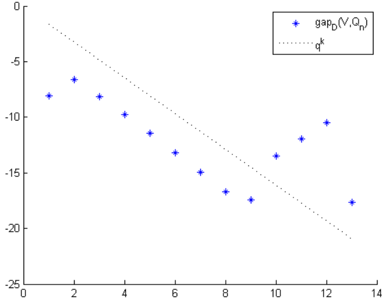
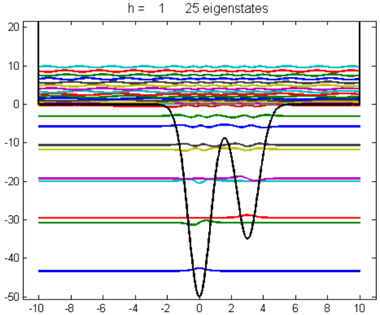


Chebfun

a Matlab implementation of FEAST + **Chebyshev** polynomial discretization – the growth of the algebraic error





When to use numerical rational calculuss

- eigenvalues of infinite multiplicity

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- indefinite operators (Maxwell,Dirac,...)

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When to use numerical rational calculuss

- eigenvalues of infinite multiplicity
- indefinite operators (Maxwell,Dirac,...)
- nonlocal operators
  - fractional differential operators
  - semi-groups
  - etc

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Thank you for your attention!