Filtered Subspace Iteration for Selfadjoint Operator Eigenvalue Problems

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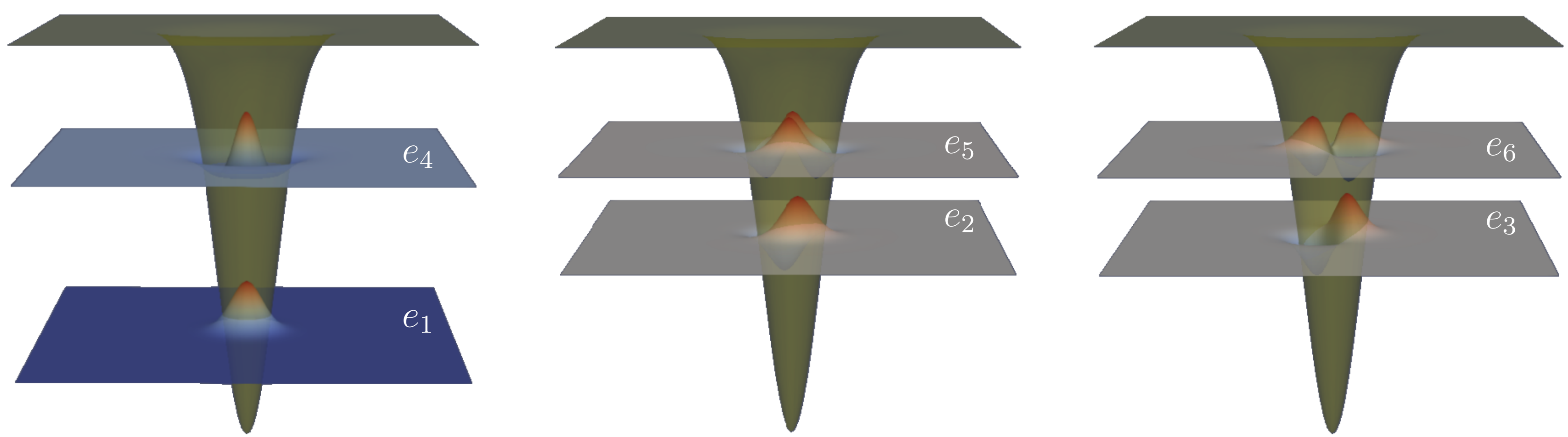


NSF DMS-1414365 and DMS-1522471

Basic Discretizations: Finite Differences

1D Model Problem (Strong Form):

$$-u'' = \lambda u \text{ in } (0,1) \quad , \quad u(0) = u(1) = 0$$

- $u_n = \sin(n\pi x)$, $\lambda_n = (n\pi)^2$, $n \in \mathbb{N}$

Finite Difference Discretization:

$$\frac{-\tilde{u}_{j-1} + 2\tilde{u}_j - \tilde{u}_{j+1}}{h^2} = \tilde{\lambda}\tilde{u}_j \text{ for } 1 \le j \le N \quad , \quad \tilde{u}_0 = \tilde{u}_{N+1} = 0$$

- Uniform grid: $h = 1/(N+1)$, $x_j = jh$, $0 \le j \le N+1$
- Taylor's theorem: $u''(x_j) = \dfrac{u(x_{j-1}) - 2u(x_j) + u(x_{j+1})}{h^2} - \dfrac{u^{(4)}(z_j)}{12}\, h^2$

$$\frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \tilde{\mathbf{u}} = \tilde{\lambda}\tilde{\mathbf{u}}$$

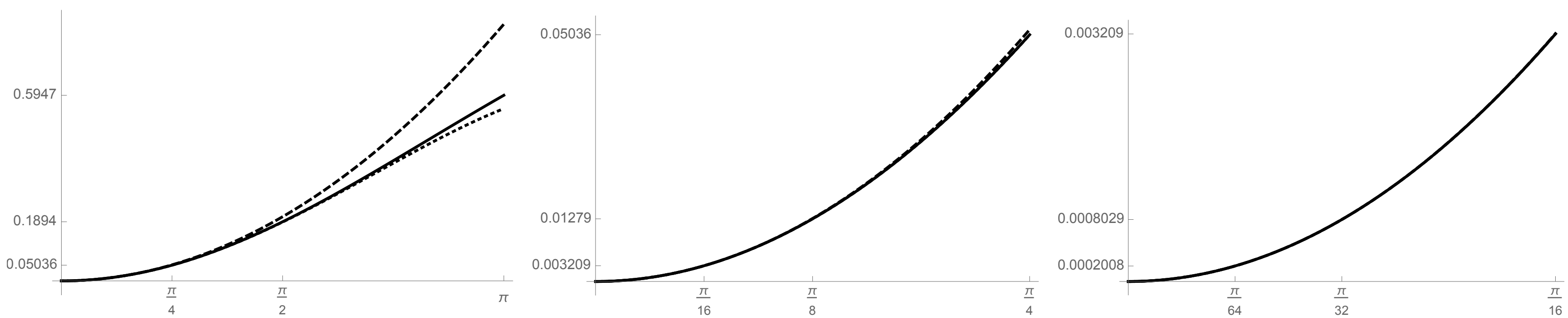
$$A\tilde{\mathbf{u}} = \tilde{\lambda}\tilde{\mathbf{u}}$$

Basic Discretizations: Finite Differences

Exact and Discrete Eigenvalues/Vectors:

- $u_n = \sin(n\pi x)$, $\lambda_n = (n\pi)^2$, $n \in \mathbb{N}$
- $\tilde{\mathbf{u}}_n = (\sin(n\pi x_1), \ldots, \sin(n\pi x_N))$, $\tilde{\lambda}_n = \frac{2-2\cos(n\pi h)}{h^2}$, $1 \le n \le N$
- Relative errors: $0 < \dfrac{\lambda_n - \tilde{\lambda}_n}{\lambda_n} = 1 - \dfrac{2-2\cos(n\pi h)}{(n\pi h)^2}$ $\qquad 0 < n\pi h < \pi$

$$\frac{x^2}{12} - \frac{x^4}{360} < 1 - \frac{2-2\cos x}{x^2} = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{2x^{2k}}{(2k+2)!} < \frac{x^2}{12}$$



Basic Discretizations: Finite Elements

1D Model Problem (Weak Form):

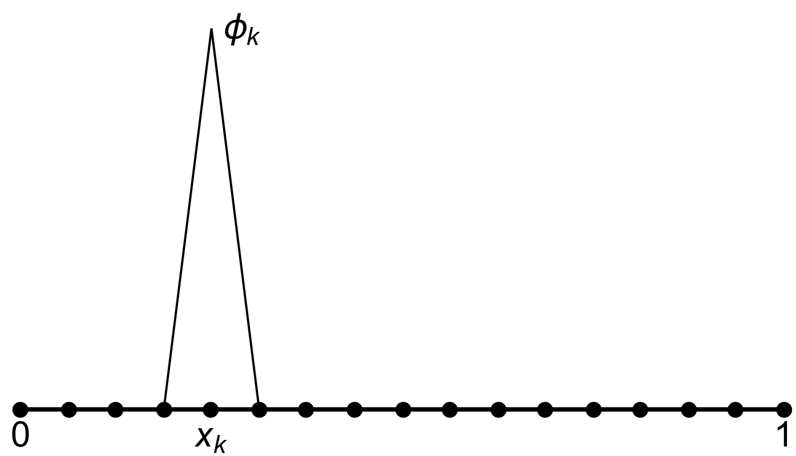
$$\int_0^1 u'v'\,dx = \lambda \int_0^1 uv\,dx \text{ for all } v \in H_0^1(0,1)$$

- Integration-by-parts, $a(u,v) = \int_0^1 u'v'\,dx$, $b(u,v) = \int_0^1 uv\,dx$

Finite Element Discretization:

$$a(\hat{u},v) = \hat{\lambda}\, b(\hat{u},v) \text{ for all } v \in V$$

- Uniform grid: $h = 1/(N+1)$, $x_j = jh$, $0 \le j \le N+1$, $I_k = [x_{k-1}, x_k]$
- $V = \{v \in C[0,1] : \; v_{|_{I_k}} \in \mathbb{P}_1(I_k)\;,\; v(0) = v(1) = 0\} = \text{span}\{\phi_1, \ldots, \phi_N\}$



Basic Discretizations: Finite Elements

Generalized (Matrix) Eigenvalue Problem:

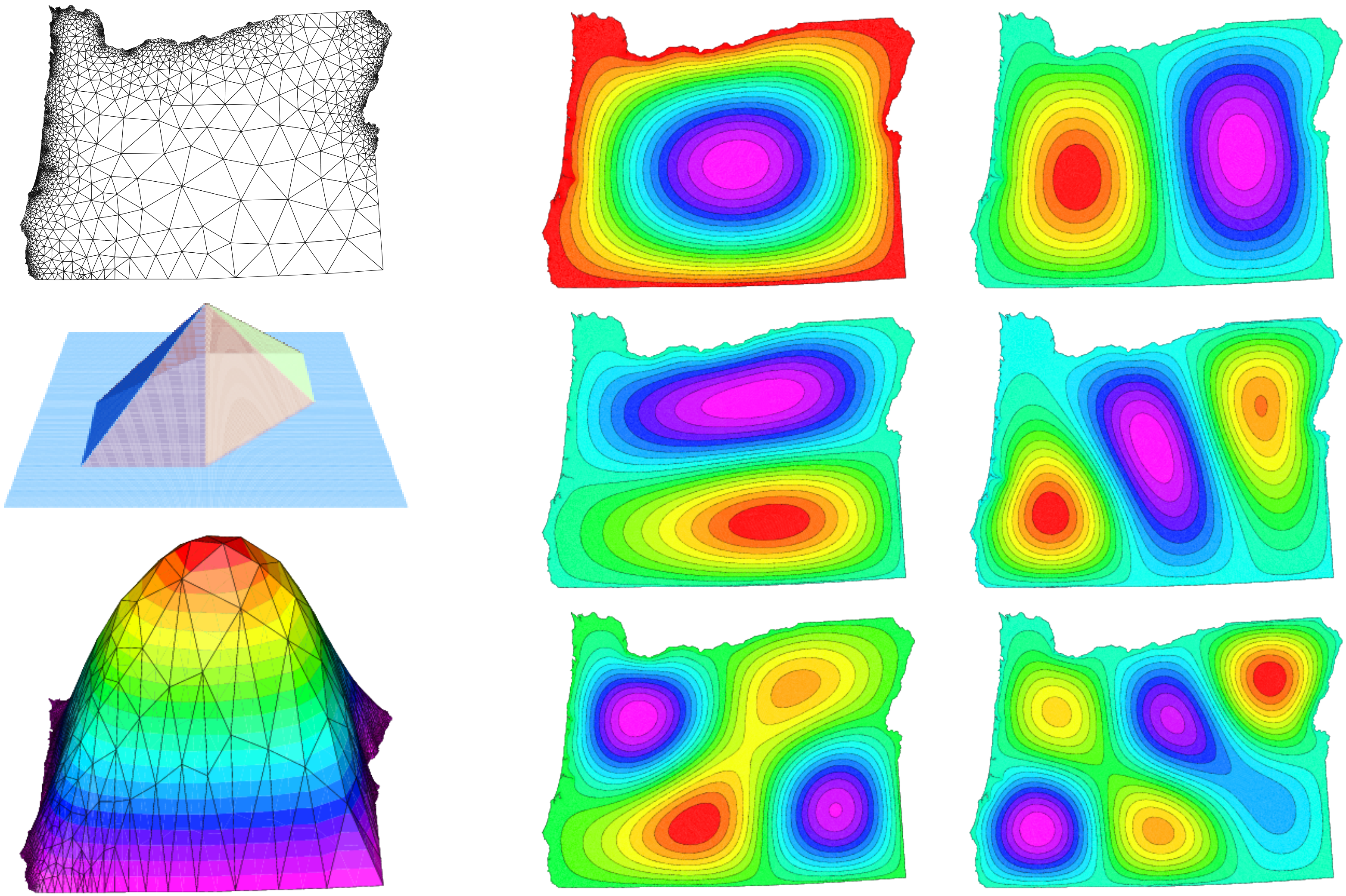
$$\frac{1}{h}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \hat{\mathbf{u}} = \hat{\lambda}\,\frac{h}{6}\begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 4 & 1 \\ & & & 1 & 4 \end{pmatrix} \hat{\mathbf{u}} \qquad A\hat{\mathbf{u}} = \hat{\lambda} B \hat{\mathbf{u}}$$

Exact and Discrete Eigenvalues/Vectors:

- $u_n = \sin(n\pi x)$, $\lambda_n = (n\pi)^2$, $n \in \mathbb{N}$
- $\hat{u}_n = \sum_{k=1}^{n} \sin(n\pi x_k)\,\phi_k$, $\hat{\lambda}_n = \frac{6}{h^2}\frac{2-2\cos(n\pi h)}{4+2\cos(n\pi h)}$, $1 \le n \le N$
- Relative errors: $0 < \dfrac{\hat{\lambda}_n - \lambda_n}{\lambda_n} = \dfrac{6}{(n\pi h)^2}\dfrac{2-2\cos(n\pi h)}{4+2\cos(n\pi h)} - 1 < 0.444 \qquad 0 < n\pi h < \pi$

$$\frac{x^2}{12} < \frac{6}{x^2}\frac{2-2\cos x}{4+2\cos x} - 1 < \frac{x^2}{12} + \frac{x^4}{360} \text{ for } 0 \le x \le 2$$

Finite Element Discretization in 2D



35.6685 , 72.4200 , 104.0508 , 131.8838 , 141.8885 , 194.9604

A Relationship Between Eigenvalue and Eigenvector Error

Variational Eigenvalue Problem: Find $\lambda \in \mathbb{R}$, non-zero $u \in \mathcal{H}$ such that

$$a(u,v) = \lambda b(u,v) \text{ for all } v \in \mathcal{H}$$

- b an inner product, assoc. norm $\|\cdot\|_b$
- a a semi-inner product, assoc. seminorm $|\cdot|_a$

A Simple Identity: (λ, u) an eigenpair, with $\|u\|_b = 1$, $\hat{u} \in \mathcal{H}$ any vector with $\|\hat{u}\|_b = 1$, $\hat{\lambda} = a(\hat{u},\hat{u})$ (Rayleigh quotient)

$$\hat{\lambda} - \lambda = |u - \hat{u}|_a^2 - \lambda \|u - \hat{u}\|_b^2$$

- "Eigenvalue error behaves like square of eigenvector error"
- Methods (e.g. finite elements) typically focus on controlling eigenvector error
- Results like this for clusters of eigenvalues, assoc. invariant subspaces?

Elements of Error Estimation

Model Problem(s): Find non-zero $u \in H_0^1(\Omega)$ and $\lambda \in \mathbb{R}$ such that

$$\underbrace{\int_\Omega D\nabla u \cdot \nabla v + ruv\,dx}_{a(u,v)} = \lambda \underbrace{\int_\Omega uv\,dx}_{b(u,v)} \text{ for all } v \in H_0^1(\Omega)$$

Given a finite dimensional subspace $V \subset H_0^1(\Omega)$, find non-zero $\hat{u} \in V$ and $\hat{\lambda} \in \mathbb{R}$ such that

$$a(\hat{u}, v) = \hat{\lambda}\, b(\hat{u}, v) \text{ for all } v \in V \quad (1)$$

- $0 < \lambda_1 < \lambda_2 \leq \cdots \quad , \quad 0 < \hat{\lambda}_1 \leq \hat{\lambda}_2 \leq \cdots \leq \hat{\lambda}_{\mathrm{dim}(V)} \quad , \quad \lambda_i \leq \hat{\lambda}_i$

Error Estimation: Let $(\hat{\lambda}_i, \hat{u}_i)$ be an eigenpair of (1), with $\|\hat{u}_i\|_b = 1$.

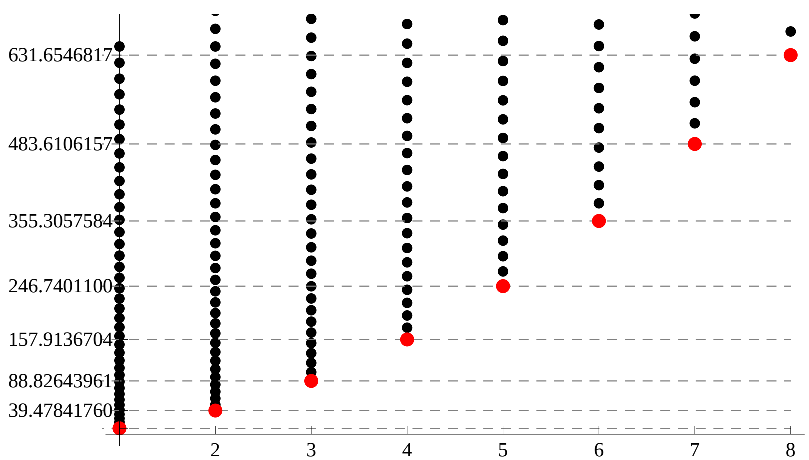
$$\inf_{u \in E(\lambda_i)} \|u - \hat{u}_i\| \leq C(\hat{\lambda}_i, \hat{\lambda}) \|u_i^* - \hat{u}_i\| \quad , \quad 0 \leq \hat{\lambda}_i - \lambda_i \leq \inf_{u \in E(\lambda_i)} \|u - \hat{u}_i\|_a^2$$

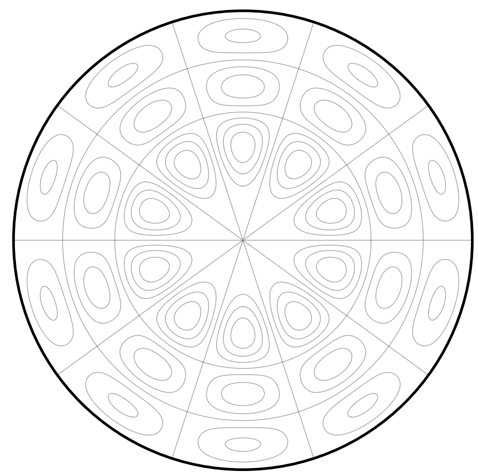
- $\|\cdot\|$ can be either a-norm or b-norm $\quad , \quad C(\hat{\lambda}_i, \hat{\lambda}) = \max_{\mu \in \mathrm{Spec} \setminus \{\lambda_i\}} \frac{\mu}{|\mu - \hat{\lambda}_i|}$
- $u_i^* \in H_0^1(\Omega)$ satisfies $a(u_i^*, v) = b(\hat{\lambda}_i \hat{u}_i, v)$ for all $v \in H_0^1(\Omega)$
- Many techniques exist for computing estimates of quantities like $\|u_i^* - \hat{u}_i\|$

Challenges: Singularities

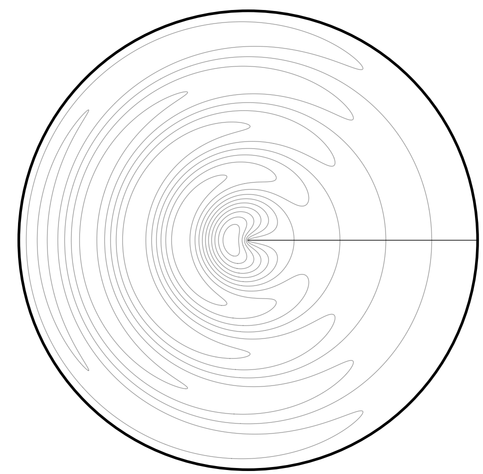
- Sector of unit disk with opening angle π/α, $\alpha \in [1/2, 1)$
- $\lambda_{m,n} = z_{m,n}^2$, $\psi_{m,n} = J_{n\alpha}(z_{m,n} r)\sin(n\alpha\theta) \sim r^{n\alpha}$
- $z_{m,n}$ is m^{th} positive root of $J_{n\alpha}$
- Singular and analytic eigenvectors interspersed throughout spectrum
- Below, slit disk ($\alpha = 1/2$); $r^{1/2}$-singularities in red

$$J_{1/2}(x) = \sqrt{\frac{2}{\pi x}}\,\sin x$$



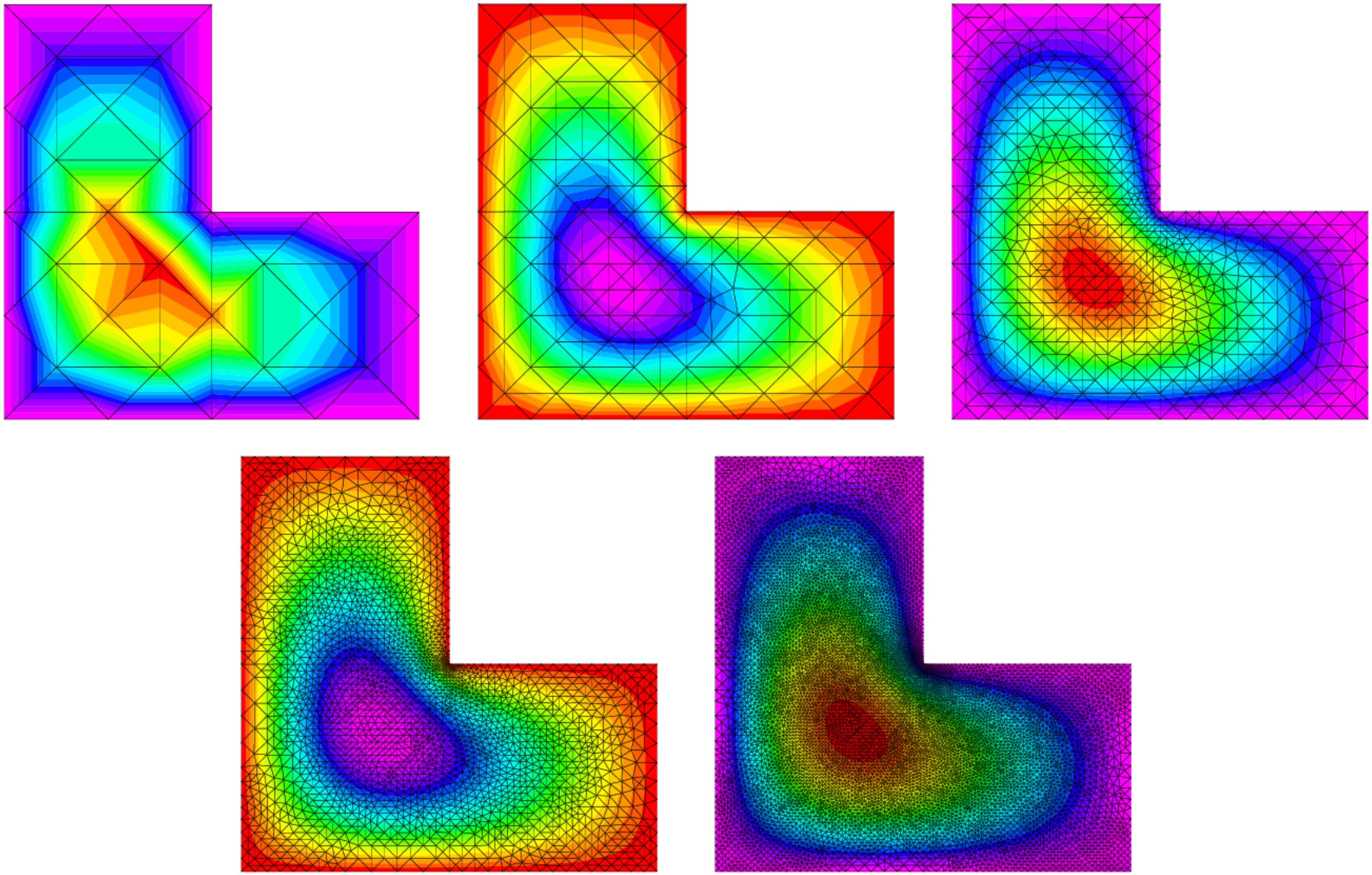


λ_{52}=246.49546613

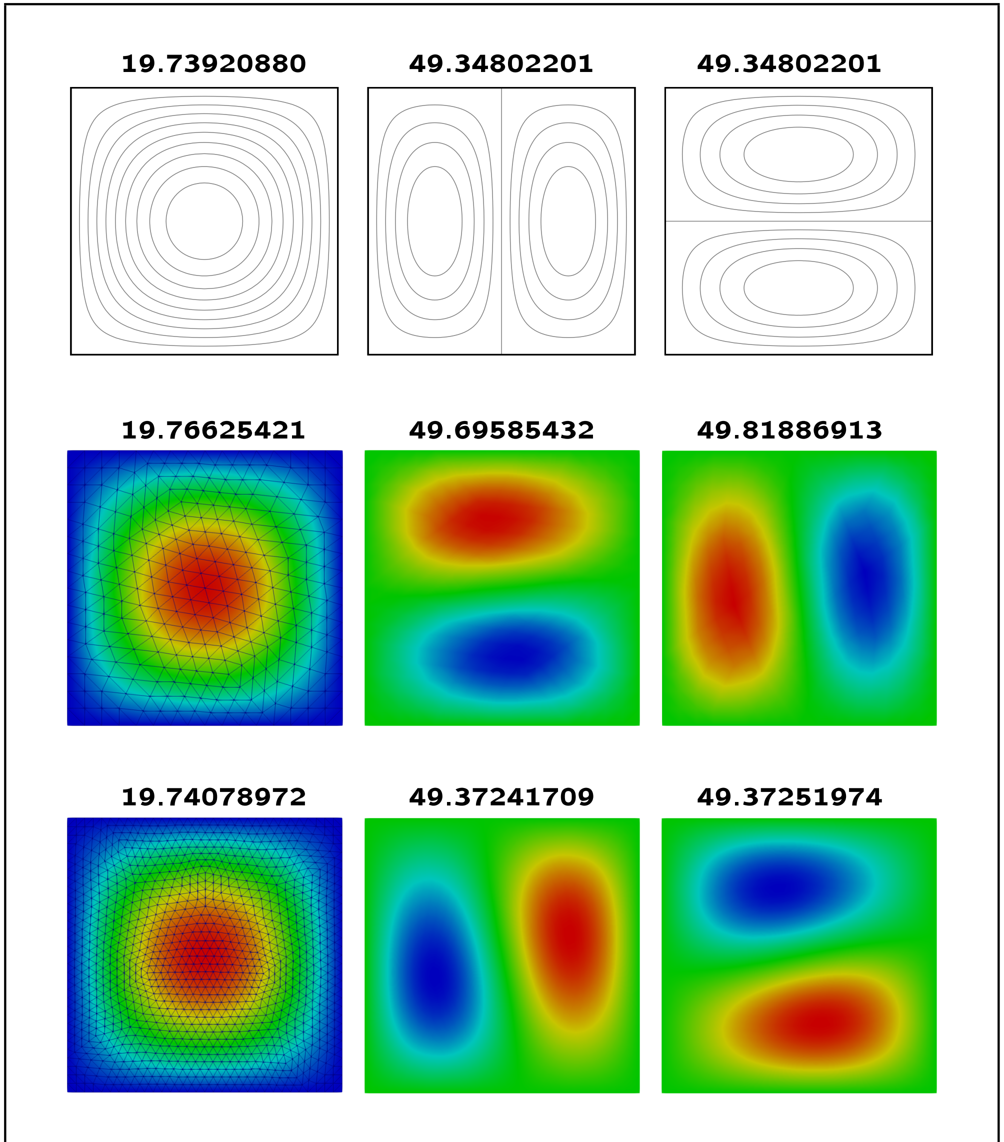


λ_{53}=246.74011003

Challenges: Singularities



Challenges: Repeated Eigenvalues



Babuška-Osborn Example

$$\phi(x) = \pi^{-\alpha}\mathrm{sign}(x)|x|^{1+\alpha}$$

$$\phi'(x) = \pi^{-\alpha}(1+\alpha)|x|^{\alpha}$$

$$-\left(\frac{u'(x)}{\phi'(x)}\right)' = \lambda\phi'(x)u(x)$$

$$u(-\pi) = u(\pi)$$

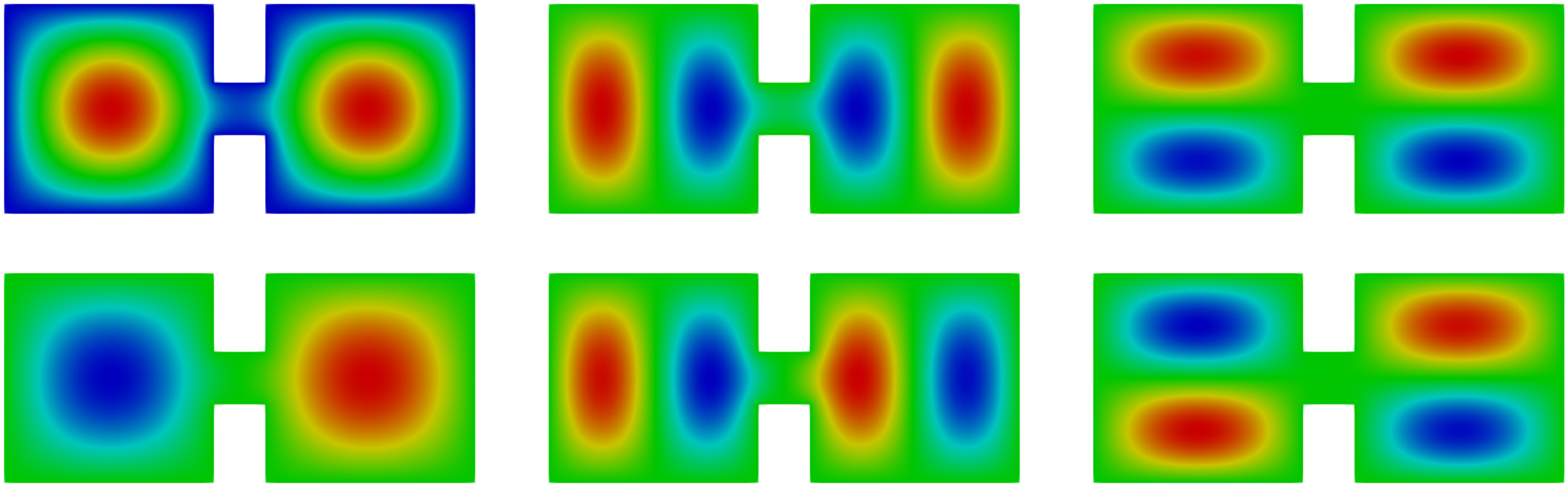
$$\frac{u'(-\pi)}{\phi'(-\pi)} = \frac{u'(\pi)}{\phi'(\pi)}$$

- $\lambda_0 = 0,\ u_0 = 1$
- $\lambda_{2n-1} = \lambda_{2n} = n^2 \qquad n \in \mathbb{N}$

$$u_{2n-1}(x) = \sin(n\phi(x))$$

$$u_{2n}(x) = \cos(n\phi(x))$$

Challenges: Clustered Eigenvalues



	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
$h = 2^{-3}$	19.318164	19.364766	47.449173	47.726913	49.320389	49.320606
$h = 2^{-4}$	19.308869	19.356441	47.408335	47.691800	49.318090	49.318225
$h = 2^{-5}$	19.305146	19.353140	47.391660	47.677648	49.317276	49.317411
$h = 2^{-6}$	19.303796	19.351947	47.385594	47.672517	49.316990	49.317126
"exact"	19.302911	19.351166	47.381613	47.669156	49.316805	49.316941

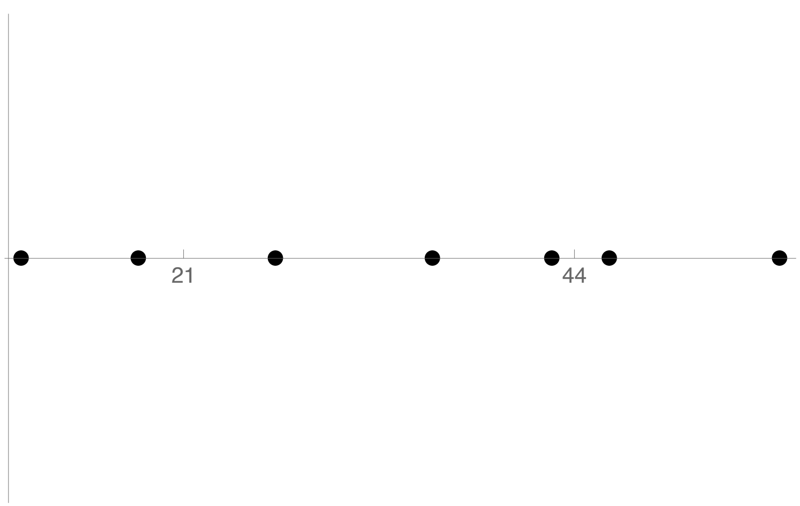
Problem of Interest

Problem of Interest: Compute "slice" of spectrum

$$\Lambda = \mathrm{spec}(A) \cap (y-\gamma, y+\gamma)$$

$$E = \mathrm{span}\{\psi \in \mathrm{dom}(A) : A\psi = \lambda\psi \text{ for some } \lambda \in \Lambda\}$$

- $A : \mathrm{dom}(A) \subset \mathcal{H} \to \mathcal{H}$ (unbounded) closed, selfadjoint operator on a Hilbert space
  e.g. $\mathcal{H} = L^2(\Omega)$, $A = -\Delta + V$
- Λ contains finitely many eigenvalues, each with finite multiplicity
- $\mathrm{spec}(A) \setminus \Lambda \subset \{x \in \mathbb{R} : |x-y| \geq (1+\delta)\gamma\}$ for some $\delta > 0$



$y = 65/2$

$\gamma = 23/2$

$\delta = 0.178512$

Filtering

Filtering

Suppose that f is real-valued, bounded and continuous on spec(A). Then $f(A) : \mathcal{H} \to \mathcal{H}$ is bounded and selfadjoint, and if $\lambda \in$ spec(A) and $A\psi = \lambda\psi$ for some $\psi \in$ dom(A), then $f(A)\psi = f(\lambda)\psi$.

Choose f so that:

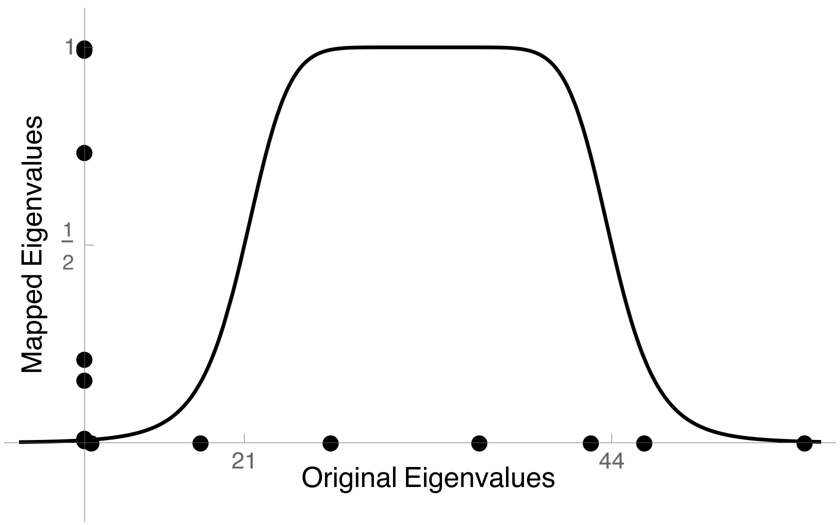
- E is dominant eigenspace of $f(A)$,

$$\min_{\lambda \in \Lambda} |f(\lambda)| > \sup_{\lambda \in \mathrm{spec}(A) \setminus \Lambda} |f(\lambda)|$$

- Action of $f(A)$ is (approx.) computable

$$f(z) = w_N + \sum_{k=0}^{N-1} w_k (z_k - z)^{-1}$$

$$f(A) = w_N + \sum_{k=0}^{N-1} w_k (z_k - A)^{-1}$$



Guidance for Selecting Filters

Cauchy's Integral Formula:

Let $\Gamma \subset \mathbb{C} \setminus \text{spec}(A)$ be a positively oriented, simple, closed contour that encloses Λ and excludes $\text{spec}(A) \setminus \Lambda$, and let $G \subset \mathbb{C}$ be the open set whose boundary is Γ. Then,

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

Spectral Projector (Ideal Filter)

$$S = r(A) = \frac{1}{2\pi i} \oint_\Gamma R(\xi) \, d\xi \quad , \quad R(z) = (z - A)^{-1} \quad , \quad E = \text{Range}(S)$$

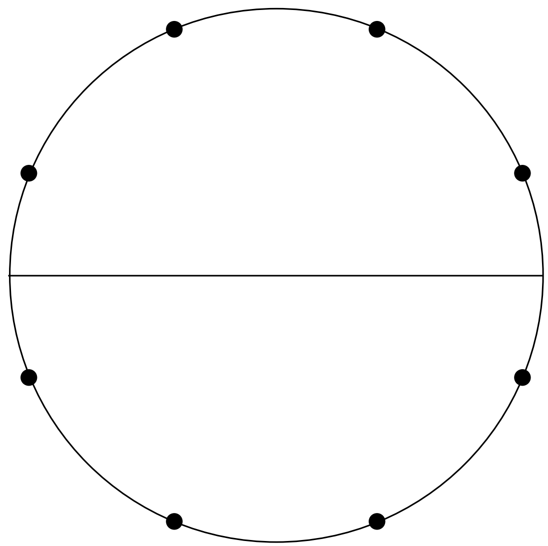
Rational Filter (Quadrature Approximation)

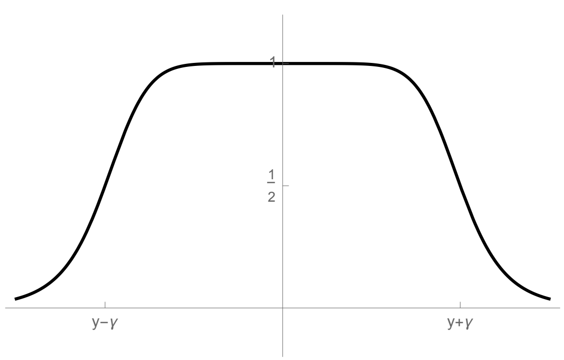
$$r_N(z) = \sum_{k=0}^{N-1} w_k (z_k - z)^{-1} \quad , \quad S_N = r_N(A) = \sum_{k=0}^{N-1} w_k R(z_k)$$

Example Filters

Circle Filter

$$r_N(z) = \frac{1}{1 + ((z-y)/\gamma)^N}$$

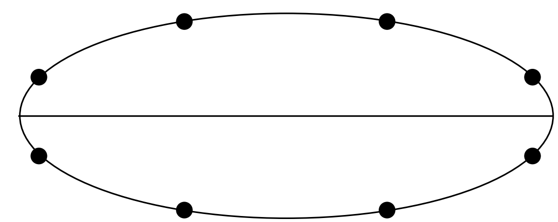


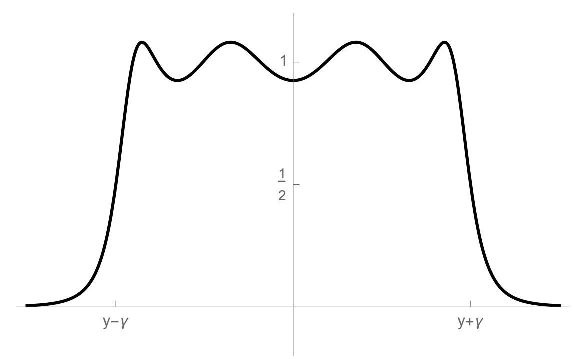


Ellipse Filter

$$r_N(z) = \frac{\frac{\rho^N - \rho^{-N}}{2}}{\frac{\rho^N + \rho^{-N}}{2} + T_N\left(\frac{\rho+\rho^{-1}}{2}\frac{z-y}{\gamma}\right)}$$

- $\rho > 1$ governs eccentricity
- Approaches circle as $\rho \to \infty$
- Approaches interval as $\rho \to 1$





Several Contour Integral Based Methods

SSM

- Sakurai/Sugiura, *A projection method for generalized eigenvalue problems using numerical integration*, J. Comput. Math. Appl. (2003)
- Sakurai/Tadano, *CIRR: A Rayleigh-Ritz type method with contour integral for generalized eigenvalue problems*, Hokkaido Math. J. (2007)
- Beyn, *An integral method for solving non-linear eigenvalue problems*, Linear Algebra Appl. (2012)
- Austin/Trefethen, *Computing eigenvalues of real symmetric matrices with rational filters in real arithmetic*, SISC (2015)

FEAST

- Polizzi, *Density-matrix-based algorithm for solving eigenvalue problems*, Phys. Rev. B (2009)
- Tang/Polizzi, *FEAST as a subspace iteration eigensolver accelerated by approximate spectral projection*, SIMAX (2014)
- Güttel/Polizzi/Tang/Viaud, *Zolotarev quadrature rules and load balancing for the FEAST eigensolver*, SISC (2015)
- Gopalakrishan/Grubišić /Ovall (2017/2018)

RIM

- Sun/Xu/Zeng, *A spectral projection method for transmission eigenvalue problem*, Science China Math. (2016)
- Huang/Struthers/Sun/Zhang, *Recursive integral method for transmission eigenvalues*, JCP (2016)

Filtered Subspace Iteration

Ideal Filtered Subspace Iteration

- Eigenspace of interest, E, is dominant eigenspace of S_N
- Let $E^{(0)} \subset \mathcal{H}$ be a (random) finite dimensional subspace such that $SE^{(0)} = E$
  - Must have $\dim(E^{(0)}) \geq \dim(E) \doteq m$; would like $\dim(E^{(0)}) = m$
- $E^{(\ell)} \approx E$ generated by subspace iteration,

$$E^{(\ell+1)} = S_N E^{(\ell)}$$

  - (Periodically) orthogonalize basis of $E^{(\ell)}$—implicitly via Rayleigh-Ritz procedure
  - $\dim(E^{(\ell)})$ paired down (if necessary) so that $\dim(E^{(\ell)}) = m$ for ℓ suff. large
- $\Lambda^{(\ell)} \approx \Lambda$ generated by Rayleigh-Ritz procedure on restriction of A to $E^{(\ell)}$

Key Questions

(In what sense) do $E^{(\ell)} \to E$ and $\Lambda^{(\ell)} \to \Lambda$? At what rates?

What are the effects of discretization, $S_N^h = \sum_{k=0}^{N-1} w_k R_h(z_k) \approx S_N$?

Iteration Error in Ideal Filtered Subspace Iteration

Iteration Error Theorem: Suppose that $SE^{(0)} = E$, and $\psi \in E$ is an eigenvector of A with eigenvalue $\lambda \in \Lambda$. There is a sequence $\{w^{(\ell)} \in E^{(\ell)} : \ell \geq 0\}$ such that

$$w^{(\ell)} - \psi = \frac{1}{[r_N(\lambda)]^\ell} S_N^\ell (I - S)(w^{(0)} - \psi)$$

$$\|w^{(\ell)} - \psi\|_{\mathcal{V}} \leq (\kappa(\lambda))^\ell \, \|w^{(0)} - \psi\|_{\mathcal{V}} \quad , \quad \kappa(\lambda) = \frac{\max\{|r_N(\mu)| : \mu \in \mathrm{Spec}(A) \setminus \Lambda\}}{|r_N(\lambda)|}$$

- Recall that $\min\{|r_N(\lambda)| : \lambda \in \Lambda\} > \max\{|r_N(\mu)| : \mu \in \mathrm{Spec}(A) \setminus \Lambda\}$
- Additional Hilbert space $\mathcal{V}$ (allows $\mathcal{V} = \mathcal{H}$)
  - $\mathcal{V}$ dense and continuously embedded in $\mathcal{H}$ (e.g. $\mathcal{V} = H_0^1(\Omega)$ in $\mathcal{H} = L^2(\Omega)$)
  - $E \subset \mathcal{V}$ and $\mathcal{V}$ invariant w.r.t. resolvent $R(z) = (z - A)^{-1}$
  - $(R(z)v, w)_{\mathcal{V}} = (v, R(\overline{z})w)_{\mathcal{V}}$ for all $v, w \in \mathcal{V}$
- Contraction factor independent of norm!
- Variants on this result allowing for subspaces generated by perturbed versions of S_N.

Illustrating the Iteration Error Theorem

Matrix Eigenvalue Problem: $A\mathrm{x} = \lambda\mathrm{x}$

- $A \in \mathbb{R}^{n\times n}$ tridiagonal w/ stencil $(-1, 2, -1)$
- Eigenvalues $\lambda_j = 2 - 2\cos(j\,\frac{\pi}{n+1})$, eigenvectors $[\boldsymbol{\psi}_j]_i = \sin(ij\,\frac{\pi}{n+1})$
- With $n = 100$, $y = 1/3$, $\gamma = 1/18$, we have $\Lambda = \{\lambda_{18}, \lambda_{19}, \lambda_{20}\}$

Eigenvalue Error:

- We compute $\{\boldsymbol{\psi}_{18}^{(\ell)}, \boldsymbol{\psi}_{19}^{(\ell)}, \boldsymbol{\psi}_{20}^{(\ell)}\}$, not $\{\mathbf{w}_{18}^{(\ell)}, \mathbf{w}_{19}^{(\ell)}, \mathbf{w}_{20}^{(\ell)}\}$ from theorem
- We compute $\lambda_j^{(\ell)} = \|\!|\boldsymbol{\psi}_j^{(\ell)}|\!\|^2 / \|\boldsymbol{\psi}_j^{(\ell)}\|^2$, where $\|\!|\mathbf{x}|\!\|^2 = \mathbf{x}^T A\mathbf{x}$, $\|\mathbf{x}\|^2 = \mathbf{x}^T\mathbf{x}$
- Eigenvalue error: $\lambda_j^{(\ell)} - \lambda_j = \|\!|\boldsymbol{\psi}_j - \boldsymbol{\psi}_j^{(\ell)}|\!\|^2 - \lambda_j\|\boldsymbol{\psi}_j - \boldsymbol{\psi}_j^{(\ell)}\|^2$
- $\mathrm{ERR} = \mathrm{ERR}(\ell) = |\lambda_j - \lambda_j^{(\ell)}|$, $\mathrm{RAT} = \mathrm{RAT}(\ell) = \mathrm{ERR}(\ell)/\mathrm{ERR}(\ell-1)$
- Hope: $\mathrm{RAT}(\ell) \sim \kappa_j^2$, can compute κ_j^2 explicitly in this case

Illustrating the Iteration Error Theorem

	$\hat{\kappa}^2$	ℓ	λ_{17} ERR	λ_{17} RAT	λ_{18} ERR	λ_{18} RAT	λ_{19} ERR	λ_{19} RAT
Circle Filter	4.773e-01	2	2.947e-04	1.961e-01	2.602e-04	1.573e-01	1.569e-03	1.848e-01
		3	3.584e-05	1.216e-01	3.109e-05	1.195e-01	2.321e-04	1.460e-01
		4	4.312e-06	**1.203e-01**	3.706e-06	1.192e-01	3.331e-05	1.435e-01
		5	5.187e-07	**1.203e-01**	4.420e-07	**1.193e-01**	4.762e-06	**1.429e-01**
		6	6.240e-08	**1.203e-01**	5.274e-08	**1.193e-01**	6.803e-07	**1.429e-01**
		7	7.507e-09	**1.203e-01**	6.293e-09	**1.193e-01**	9.718e-08	**1.429e-01**
Ellipse Filter	1.563e-01	2	5.844e-05	3.820e-02	1.408e-04	4.163e-02	4.597e-04	5.512e-02
		3	2.243e-06	3.838e-02	6.015e-06	4.272e-02	1.917e-05	4.171e-02
		4	8.627e-08	3.846e-02	2.576e-07	**4.283e-02**	7.900e-07	4.120e-02
		5	3.319e-09	**3.847e-02**	1.103e-08	**4.283e-02**	3.254e-08	**4.118e-02**
		6	1.277e-10	**3.847e-02**	4.726e-10	**4.283e-02**	1.340e-09	**4.118e-02**
		7	4.910e-12	**3.847e-02**	2.024e-11	**4.283e-02**	5.518e-11	**4.118e-02**

Discretization Error Theorem

Theorem: Suppose that $E_h^{(\ell+1)} = S_N^h E_h^{(\ell)}$ for $\ell \geq 0$, $P_h = \frac{1}{2\pi \mathbf{i}} \oint_\Theta (z - S_N^h)^{-1}\, dz$, and $\dim(E_h^{(0)}) = \dim(P_h E_h^{(0)}) = \dim(E)$, There is an $h_0 > 0$ such that, for $0 < h < h_0$, the subspace iterates $E_h^{(\ell)}$ converge (in gap) to $E_h = \mathrm{Range}(P_h)$. Furthermore,

$$\mathrm{gap}_{\mathcal{V}}(E, E_h) \leq C h^{\min(p, s_E)} \quad , \quad \mathrm{dist}(\Lambda, \Lambda_h) \leq C h^{2\min(p, s_E)}$$

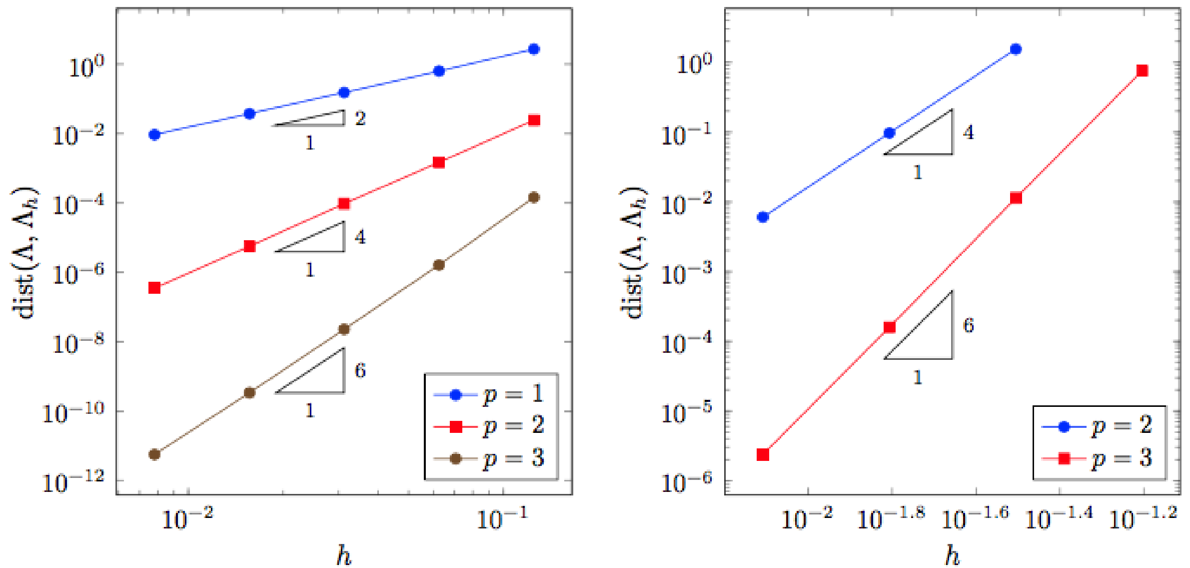
- $\mathcal{V} = H^1(\Omega)$, A a Laplace-like operator
- h mesh-size, p polynomial degree
- s_E (worst-case) regularity index for functions in E
- Hausdorff distance between sets of numbers X, Y

$$\mathrm{dist}(X, Y) = \max\left[\sup_{x\in X} \inf_{y \in Y} |x - y| \, , \, \sup_{y \in Y} \inf_{x\in X} |x - y|\right]$$

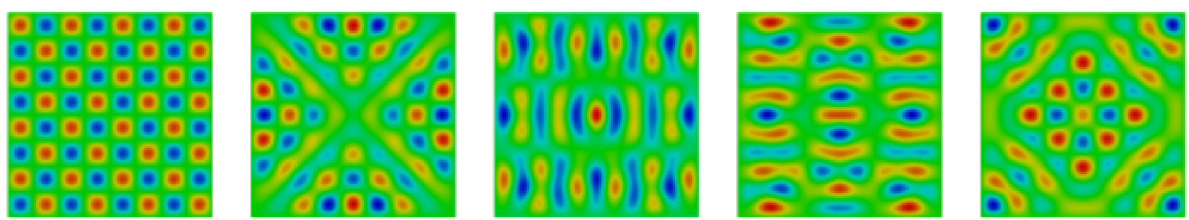
- Gap between subspaces X and Y

$$\mathrm{gap}_{\mathcal{V}}(X, Y) = \max\left[\sup_{x\in X} \inf_{y \in Y} \frac{\|x - y\|_{\mathcal{V}}}{\|x\|_{\mathcal{V}}} \, , \, \sup_{y \in Y} \inf_{x\in X} \frac{\|x - y\|_{\mathcal{V}}}{\|y\|_{\mathcal{V}}}\right]$$

Dirichlet Laplace on Unit Square



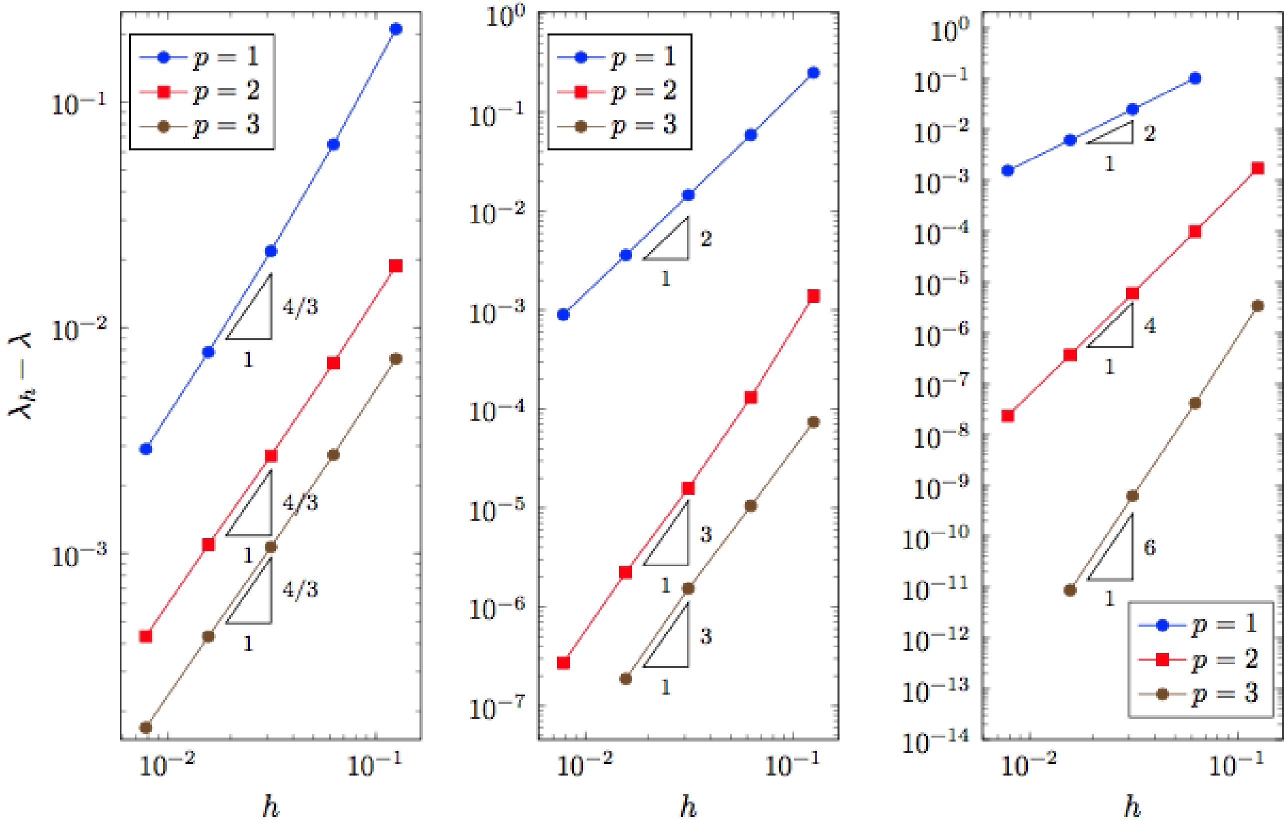
(A) Convergence rates for $\Lambda = \{2\pi^2, 5\pi^2\}$. (B) Convergence rates for $\Lambda = \{128\pi^2, 130\pi^2\}$.



FEAST Implementation

- **Gopalakrishnan.** ***Pythonic FEAST*****.** `https://bitbucket.org/jayggg/pyeigfeast`
- **Schöberl.** ***NGSolve*****.** `http://ngsolve.org`

Dirichlet Laplace on L-Shape



(A) Convergence rates for $\lambda_1 \approx 9.6397238$.

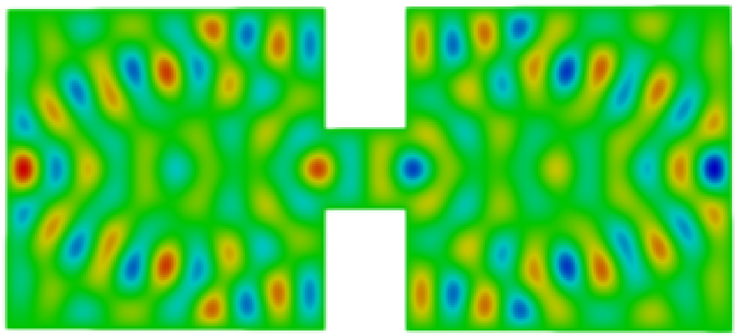
(B) Convergence rates for $\lambda_2 \approx 15.197252$.

(C) Convergence rates for $\lambda_3 = 2\pi^2$.

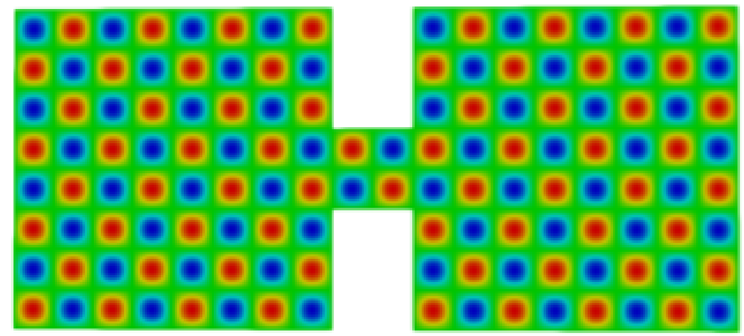
- Individual eigenvalue convergence rates in accordance corresponding eigenvector regularities, not (worst-case) cluster regularity

Dirichlet Laplace on Dumbbell

Search Interval $(1262, 1264)$**,** $p = 3$



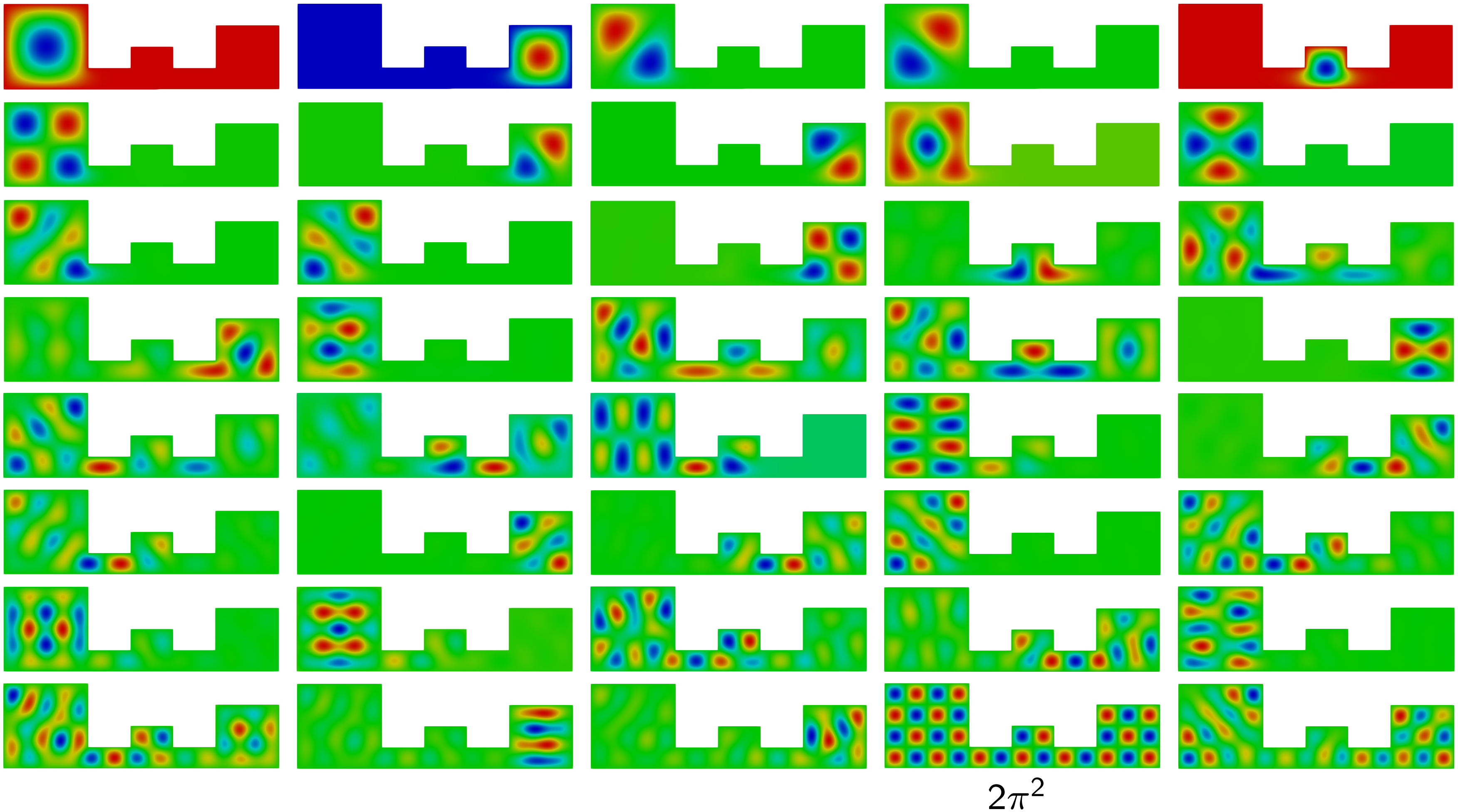
≈ 1262.41



$128\pi^2$

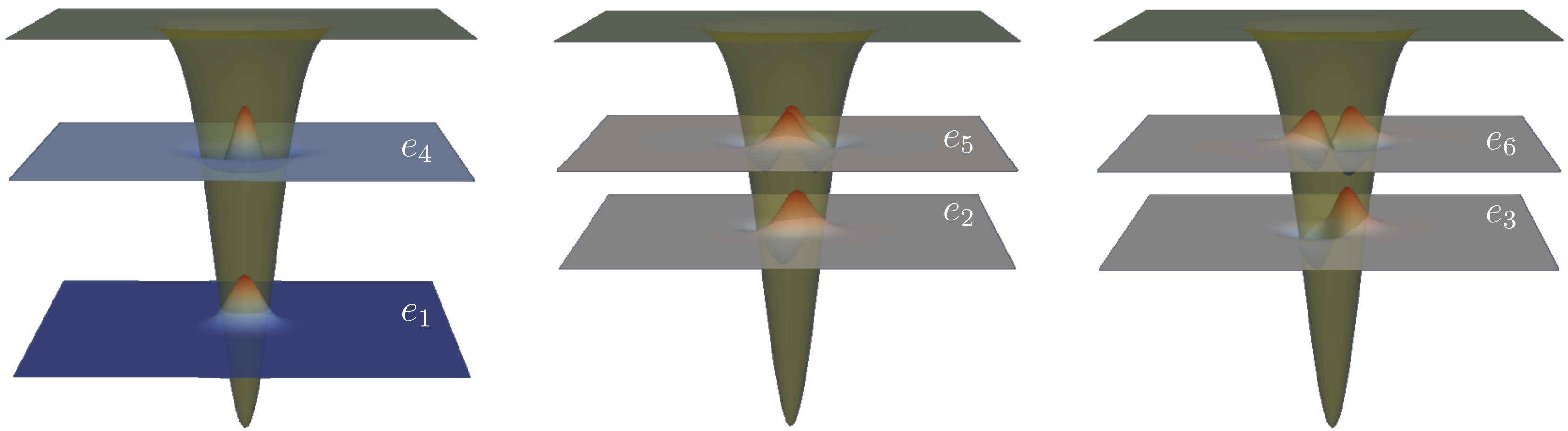
h	λ_1	λ_2
2^{-4}	1263.178867	$\underline{126}4.020566$
2^{-5}	1262.447629	$\underline{1263.3}19956$
2^{-6}	1262.418298	$\underline{1263.309}521$
2^{-7}	1262.410062	$\underline{1263.30936}6$

Dirichlet Laplace on "Three Bulb" Domain, Localization



Schrödinger Operator on $\mathcal{H} = L^2(\mathbb{R}^2)$

$$-\Delta\psi - 50e^{-(x^2+y^2)}\psi = \lambda\psi \text{ in } \mathbb{R}^2$$



p	D	λ_1^{sch}	λ_2^{sch}	λ_3^{sch}	λ_4^{sch}	λ_5^{sch}	λ_6^{sch}
4	5	−36.8759926	−24.8609439	−24.8609244	−15.1384305	−14.0895444	−14.0894693
5	5	−36.8760274	−24.8609749	−24.8609736	−15.1388526	−14.0897524	−14.0897520
6	5	−36.8760276	−24.8609775	−24.8609775	−15.1388553	−14.0897540	−14.0897540
7	5	−36.8760276	−24.8609775	−24.8609775	−15.1388555	−14.0897541	−14.0897541
7	10	−36.8760276	−24.8609775	−24.8609775	−15.1388555	−14.0897541	−14.0897541

- Spec$(A) \subset (-50, \infty)$, EssSpec$(A) = [0, \infty)$

Some Technical Details

$$S_N = \sum_{k=0}^{N-1} w_k R(z_k) \quad , \quad S_N^h = \sum_{k=0}^{N-1} w_k R_h(z_k)$$

Limit Space: Existence of limit space E_h assumes

$$\lim_{h\to 0} \|R_h(z_k) - R(z_k)\|_{\mathcal{V}} = 0 \text{ for } 0 \le k \le N-1$$

Resolvent Estimates for Eigenvalue/Vector Convergence Theorem: For each z in resolvent set of A, there are $C, h_0 > 0$ such that, for all $h < h_0$,

$$\|R(z) - R_h(z)\|_{\mathcal{V}} \le Ch^r \quad , \quad \|[R(z) - R_h(z)]_{|E}\|_{\mathcal{V}} \le Ch^{r_E}$$

$$\|R(z) - R_h(z)\|_{\mathcal{H}} \le Ch^{2r} \quad , \quad \|[R(z) - R_h(z)]_{|E}\|_{\mathcal{H}} \le Ch^{r+r_E}$$

where $r = \min(s, p)$, $r_E = \min(s_E, p)$.

Eigenvalue Discretization Error: If $\|u\|_{\mathcal{V}} = \||A|^{1/2}u\|_{\mathcal{H}}$, then

$$\text{dist}(\Lambda, \Lambda_h) \le (\Lambda_h^{\max})^2 \text{gap}_{\mathcal{V}}(E, E_h)^2 + C_0\|A_E\| \text{gap}_{\mathcal{H}}(E, E_h)^2$$

Different Classifications within Spectrum

- Resolvent Set: $\text{Res}(A) = \{z \in \mathbb{C} : z - A : \text{dom}(A) \to \mathcal{H} \text{ is bijective}\}$ open set
- Spectrum: $\text{Spec}(A) = \mathbb{C} \setminus \text{Res}(A)$ closed set
  1. Point Spectrum (Eigenvalues): $\text{Spec}_p(A) = \{\lambda \in \mathbb{C} : z - A \text{ is not injective}\}$
  2. Residual Spectrum: $\text{Spec}_r(A) = \{\lambda \in \mathbb{C} : z - A \text{ is injective, but } \overline{\text{Ran}(z - A)} \neq \mathcal{H}\}$
  3. Continuous Spectrum:
     $\text{Spec}_c(A) = \{\lambda \in \mathbb{C} : z - A \text{ is injective, and } \overline{\text{Ran}(z - A)} = \mathcal{H} \text{ but } \text{Ran}(z - A) \neq \mathcal{H}\}$

$$\text{Spec}(A) = \text{Spec}_p(A) \cup \text{Spec}_r(A) \cup \text{Spec}_c(A)$$

Some authors define $\text{Spec}_c(A)$ slightly differently, allowing $\text{Spec}_r(A) \cap \text{Spec}_c(A) \neq \emptyset$

- Discrete Spectrum: Eigenvalues of finite multiplicity that are isolated points of $\text{Spec}(A)$
- Essential Spectrum: Complement of discrete spectrum in $\text{Spec}(A)$
- If A has compact resolvent, then its spectrum, point spectrum and discrete spectrum are the same
- $\text{Spec}(A) \neq \emptyset$ (for normal operators)