Bounds and Error Estimates for Nonlinear Eigenvalue Problems

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Outline

Resonances via nonlinear eigenproblems

Sensitivity and backward error analysis

Resonances via Perfectly Matched Layers

Perturbation bounds

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Simple 1D Problem

Consider 1D Schrödinger (V nice, $\mathrm{supp}(V) \subset [a, b]$):

$$H\psi = \left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

- H self-adjoint with discrete spectrum on $E < 0$, continuous spectrum on $E \geq 0$.
- Continuous spectrum is a branch cut for the resolvent. (Think $\chi(H - E)^{-1}\chi$, χ a smooth cutoff, $\chi([a, b]) = 1$. One moral analogue of a spectral Schur complement.)
- Second-sheet poles of the resolvent are *resonances*. Correspond to trapping, quasi-stable states.

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

How do we:

1. Quickly compute resonances (nice enough V)?
2. Make sure the computations are correct?

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

If $\mathrm{supp}(V) \subset [a, b]$, write

$$\left(-\frac{d^2}{dx^2} + V(x) - k^2\right)\psi = 0, x \in (a, b)$$
$$\left(\frac{d}{dx} - ik\right)\psi = 0, x = b$$
$$\left(\frac{d}{dx} + ik\right)\psi = 0, x = a$$

$E = k^2$, $\operatorname{Im} k \geq 0$ for eigenvalues, $\operatorname{Im} k < 0$ for resonances.

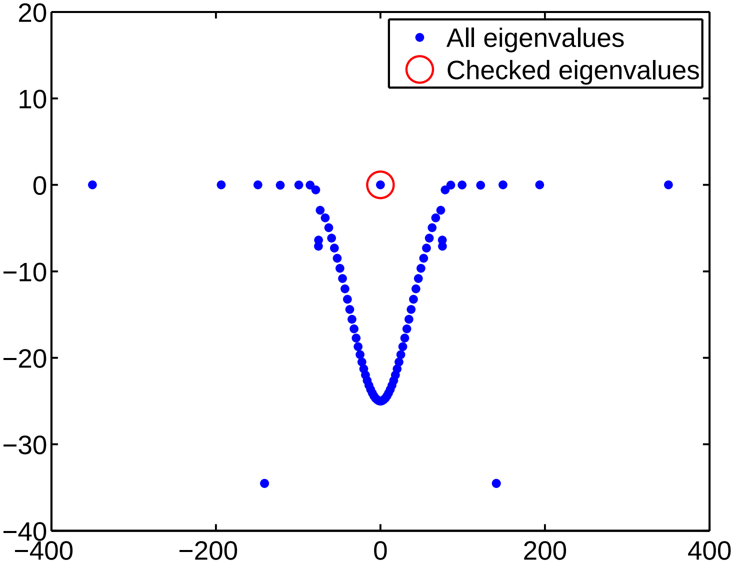
Pseudospectral Discretization

Sample ψ at Chebyshev nodes and approximate $d\psi/dx$ by differentiating the interpolant:

$$\left(-D^2 + V(x) - k^2\right)\psi = 0, x \in (a, b)$$
$$(D - ik)\psi = 0, x = b$$
$$(D + ik)\psi = 0, x = a$$

Now linearize (introduce auxiliary variable $\phi = k\psi$) to get an ordinary generalized eigenvalue problem.

Is it that easy?



Outline

Backward Error Analysis

1. If $(\hat{\psi}, \hat{E})$ is a numerical solution with above scheme, then there is some $\hat{V}$ s.t. for $x \in (a, b)$,

$$(H_{\hat{V}} - \hat{E})\hat{\psi} = \left(-\frac{d^2}{dx^2} + \hat{V}(x) - \hat{E}\right)\hat{\psi} = 0$$

   together with corresponding radiation conditions.
2. Estimate $\hat{V}$ explicitly by remapping residual to finer mesh
3. Original problem is a perturbation of computed problem.
4. Use first-order perturbation theory to correct $\hat{E}$.
   Useful to take a *variational* approach.

More General Picture

Consider Schrödinger with compactly supported V in R^d.
For E in resolvent set on appropriate Riemann surface, seek

$$\begin{aligned} (H_V - E)\psi &= f \text{ on } \Omega \\ \frac{\partial \psi}{\partial n} - B(E)\psi &= 0 \text{ on } \Gamma \end{aligned}$$

where $B(E)$ is the Dirichlet-to-Neumann map on $\partial\Omega$.
Solutions are stationary points for

$$\begin{aligned} I(\psi) &= \frac{1}{2}\int_\Omega \left((\nabla\psi)^T(\nabla\psi) + \psi(V-E)\psi\right) d\Omega + \\ &\quad \frac{1}{2}\int_\Gamma \psi B(E)\psi \, d\Gamma - \int_\Omega \psi f \, d\Omega. \end{aligned}$$

Variational Formulation

Check variational formulation:

$$I(\psi) = \frac{1}{2}\int_\Omega \Big((\nabla\psi)^T(\nabla\psi) + \psi(V-E)\psi\Big)\, d\Omega - \frac{1}{2}\int_\Gamma \psi B(E)\psi\, d\Gamma - \int_\Omega \psi f\, d\Omega.$$

Use symmetry of form (note $\int_\Gamma \phi B(E)\psi = \int_\Gamma \psi B(E)\phi$) + integration by parts:

$$\delta I(\psi) = \int_\Omega \delta\psi\,(-\Delta\psi + (V-E)\psi - f)\, d\Omega + \int_\Gamma \delta\psi\left(\frac{\partial\psi}{\partial n} - B(E)\right)\psi\, d\Gamma.$$

Rayleigh Quotient Analogue

Now define a residual for an approximate eigenpair:

$$r(\psi, E) = \int_\Omega \left((\nabla\psi)^T(\nabla\psi) + \psi(V - E)\psi \right) - \int_\Gamma \psi B(E)\psi.$$

Take variations and use symmetry of B:

$$\begin{aligned} \delta r(\psi, E) &= 2\int_\Omega \delta\psi \left[(-\Delta + V - E)\psi\right] + \\ &\quad 2\int_\Gamma \delta\psi \left[\frac{\partial\psi}{\partial n} - B(E)\psi\right] + \\ &\quad \delta E \left[\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi\right] \end{aligned}$$

For an eigenpair or resonance, $r(\psi, E) = 0$ and $\delta r(\psi, E) = 0$.

Rayleigh Quotient Analogue

We now implicitly define a differentiable function $\tilde{E}(\phi)$ in the neighborhood of an eigenpair (ψ, E), with $r(\phi, E(\phi)) = 0$ and $\tilde{E}(\psi) = E$. Such a function should exist if

$$\int_{\Omega} \psi^2 - \int_{\Gamma} \psi B'(E) \psi \neq 0$$

Stationary precisely when (ψ, E) an eigenpair.

Sensitivity

Now assume δV a compactly-supported perturbation, and look at effect of δV on Rayleigh quotient analogue. Gives that isolated eigenvalues change like

$$\delta E = \frac{\int_\Omega \delta V \psi^2}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi}$$

Can also write in terms of a residual for ψ as a solution for the potential $V + \delta V$:

$$\delta E = \frac{\int_\Omega \psi(-\Delta + (V + \delta V) - E)\psi}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi}.$$

Backward Error Analysis Revisited

1. Compute approximate solution $(\hat{\psi}, \hat{E})$.
2. Map $\hat{\psi}$ to high-resolution quadrature grid to evaluate

$$\delta E = \frac{\int_\Omega \hat{\psi}(-\Delta + V - \hat{E})\hat{\psi}}{\int_\Omega \hat{\psi}^2 - \int_\Gamma \hat{\psi} B'(\hat{E})\hat{\psi}}.$$

3. If δE large, discard $\hat{E}$ as spurious; otherwise, accept $E \approx \hat{E} + \delta E$.

Some Computational Issues

In general, using the domain equation + DtN map to find resonances is problematic because:

1. The DtN map is nonlocal, expensive to work with computationally.
2. The Green's function (and hence the DtN map) are hard to compute for some problems I care about (e.g. elastic half space problems).
3. Nonlinear eigenvalue problems are trickier than linear problems to solve.

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Perfectly Matched Layers

For scattering computations / resonance computations, need an outgoing BC. We use *perfectly matched layers*:

- Complex coordinate transformation
- Generates a “perfectly matched” absorbing layer
- Rotates the continuous spectrum to reveal resonances
- Idea works with general linear wave equations
    - Electromagnetics (Berengér, 1994)
    - Quantum mechanics – *exterior complex scaling* (Simon, 1979 – originally used to *define* resonances)
    - Elasticity in standard finite element framework (Basu and Chopra, 2003)

Model Problem

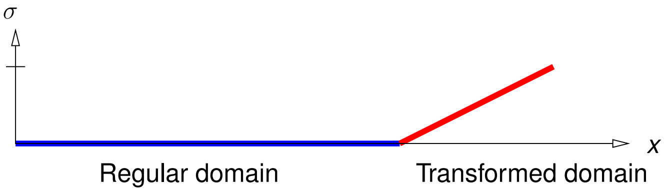
- Domain: $x \in [0, \infty)$
- Frequency-domain equation:

$$\frac{d^2 \hat{u}}{dx^2} + k^2 \hat{u} = 0$$

- Solution:

$$\hat{u} = c_{\text{out}} e^{-ikx} + c_{\text{in}} e^{ikx}$$

Model with Perfectly Matched Layer

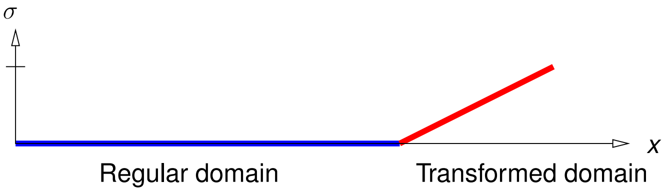


$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

$$\frac{d^2\hat{u}}{d\tilde{x}^2} + k^2\hat{u} = 0$$

$$\hat{u} = c_{\text{out}} e^{-ik\tilde{x}} + c_{\text{in}} e^{ik\tilde{x}}$$

Model with Perfectly Matched Layer



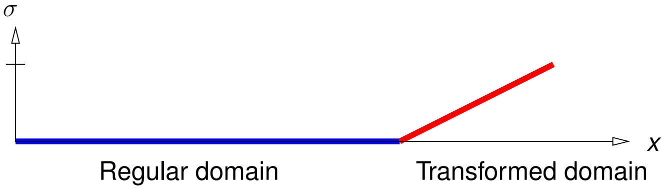
$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

$$\frac{1}{\lambda}\frac{d}{dx}\left(\frac{1}{\lambda}\frac{d\hat{u}}{dx}\right) + k^2\hat{u} = 0$$

$$\hat{u} = c_{\text{out}}e^{-ikx-k\Sigma(x)} + c_{\text{in}}e^{ikx+k\Sigma(x)}$$

$$\Sigma(x) = \int_0^x \sigma(s)\,ds$$

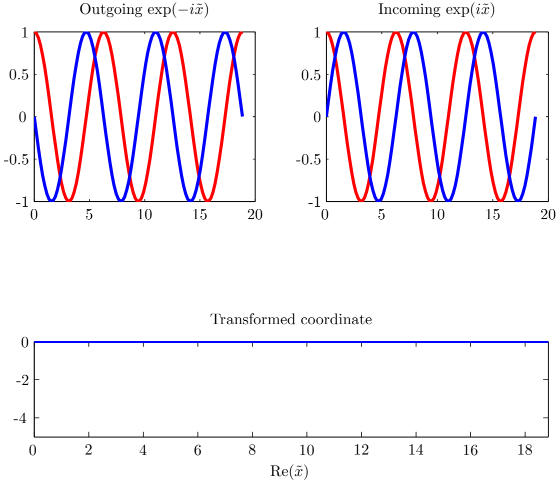
Model with Perfectly Matched Layer



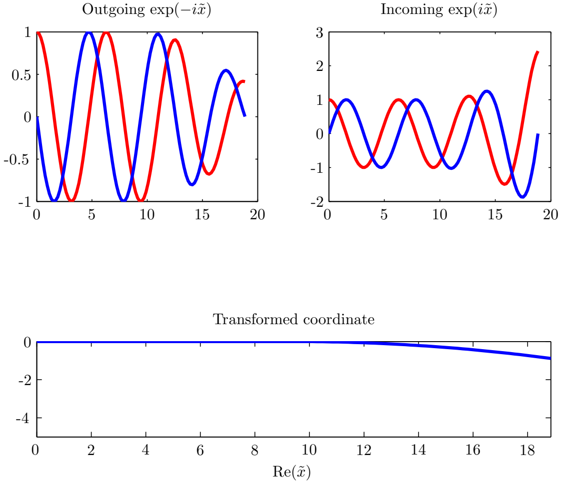
If solution clamped at $x = L$ then

$$\frac{c_{\text{in}}}{c_{\text{out}}} = O(e^{-k\gamma}) \text{ where } \gamma = \Sigma(L) = \int_0^L \sigma(s)\, ds$$

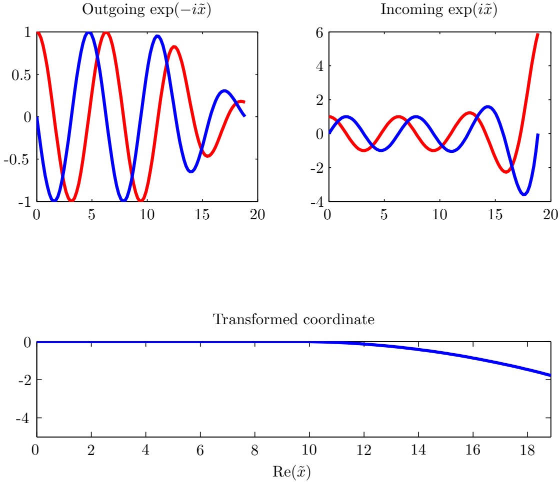
Model Problem Illustrated



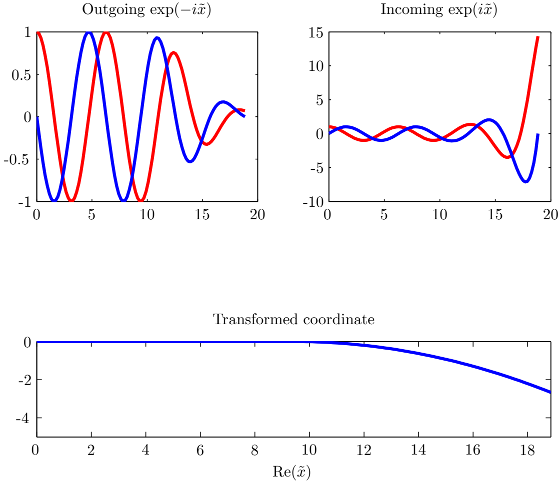
Model Problem Illustrated



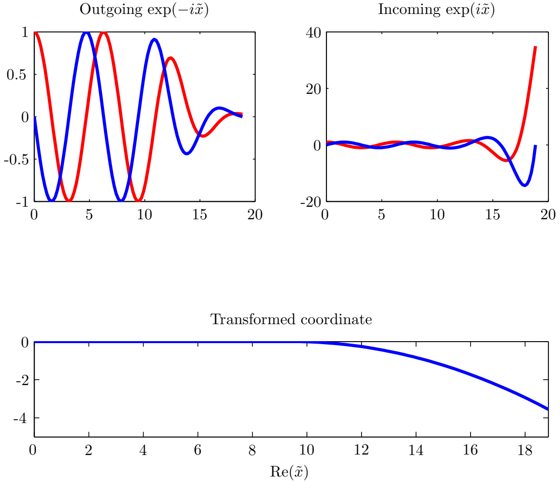
Model Problem Illustrated



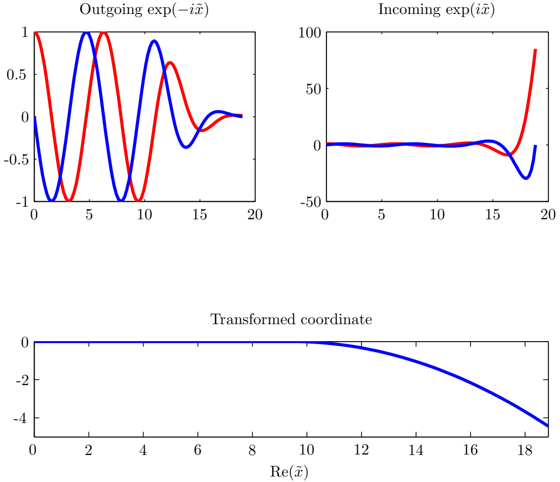
Model Problem Illustrated



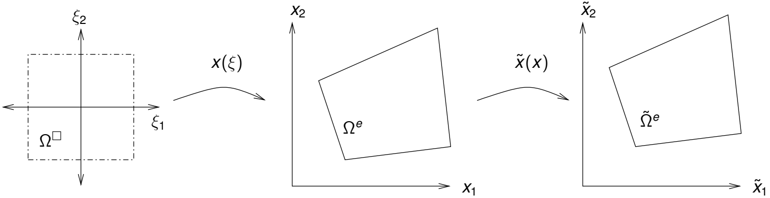
Model Problem Illustrated



Model Problem Illustrated



Finite/Spectral Element Implementation



- Combine PML and isoparametric mappings

$$\mathbf{k}^e_{ij} = \int_{\Omega^\square} (\tilde{\nabla} N_i)^T \mathbf{D} (\tilde{\nabla} N_j) \tilde{J} \, d\Omega^\square$$

$$\mathbf{m}^e_{ij} = \int_{\Omega^\square} \rho N_i N_j \tilde{J} \, d\Omega^\square$$

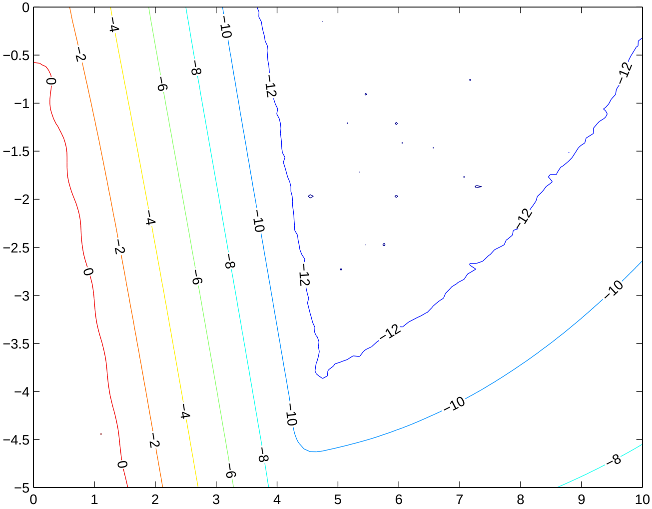
- Matrices are *complex symmetric*

DtN Approximation in PML

- Earlier (DtN) form - Neumann form = DtN term $\int_\Gamma \psi B \psi$.
- Eliminate PML dofs - Neumann form $\approx$ DtN term
- Approximation is rational in k, good locally
- Would like to understand how good approximation to DtN + some form of stability leads to error bounds.

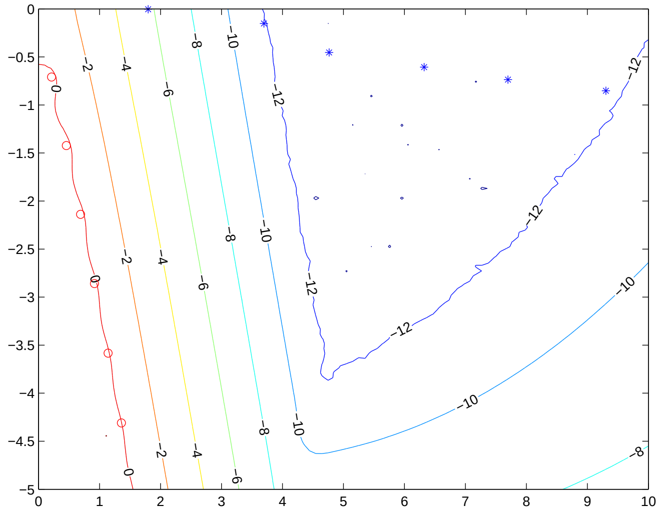
DtN Approximation in PML

$\log_{10}|B(k)_{PML} - B(k)|$ on circle of radius 3 in $\mathbb{R}^2$.
Order 30 spectral elements, PML goes $[3, 4]$.



DtN Approximation in PML

Axisymmetric resonances for ring barrier for $r \in [1, 2]$.
Stars for small residual; circles for spurious resonance.



Relation of PML to DtN Approach

- Numerically eliminate variables in PML $\Longrightarrow$ local (in k or E) rational approximation to DtN-like condition.
- Could also form explicit Padé approximation.
- Approximation is local in k – where can we guarantee (for example) that we have approximated all resonances?

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General NEP Picture

$A : \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$ analytic in Ω

$$\begin{aligned} \Lambda(A) &:= \{z \in \mathbb{C} : A(z) \text{ singular}\} \\ \Lambda_\epsilon(A) &:= \{z \in \mathbb{C} : \|A(z)^{-1}\| \geq \epsilon^{-1}\} \end{aligned}$$

- Resonance calculation with DtN map or with eliminated PML as an example.
- $\Lambda(A)$ and $\Lambda_\epsilon(A)$ describe asymptotics, transients of some linear differential or difference equation.
- Lots of function theoretic proofs from analyzing ordinary eigenvalue problems carry over without change.

Counting Eigenvalues

If A nonsingular on Γ, analytic inside, count eigs inside by

$$\begin{aligned} W_\Gamma(\det(A)) &= \frac{1}{2\pi i} \int_\Gamma \frac{d}{dz} \ln \det(A(z))\, dz \\ &= \operatorname{tr}\left(\frac{1}{2\pi i} \int_\Gamma A(z)^{-1} A'(z)\, dz \right) \end{aligned}$$

Suppose E also analytic inside Γ. By continuity,

$$W_\Gamma(\det(A)) = W_\Gamma(\det(A + sE))$$

for s in neighborhood of 0 such that $A + sE$ remains nonsingular on Γ.

Function Theoretic Perturbation Recipe

Winding number counts give continuity of eigenvalues $\Longrightarrow$
Should consider eigenvalues of $A + sE$ for $0 \leq s \leq 1$:

Analyticity of A and E +
Matrix nonsingularity test for $A + sE$ =

Inclusion region for $\Lambda(A + E)$ +
Eigenvalue counts for connected components of region

Example: Matrix Rouché

$\|A^{-1}(z)E(z)\| < 1$ on $\Gamma \implies$ same eigenvalue count in Γ

Proof:
$\|A^{-1}(z)E(z)\| < 1 \implies A(z) + sE(z)$ invertible for $0 \leq s \leq 1$.

(Gohberg and Sigal proved a more general version in 1971.)

Example: Nonlinear Gershgorin

Define

$$G_i = \left\{ z : |a_{ii}(z)| < \sum_{j \neq i} |a_{ij}(z)| \right\}$$

Then

1. $\Lambda(A) \subset \cup_i G_i$
2. Connected component $\cup_{i=1}^m G_i$ contains m eigs (if bounded and disjoint from $\partial\Omega$)

Proof: Write $A = D + F$ where $D = \mathrm{diag}(A)$.
$D + sF$ is diagonally dominant (so invertible) off $\cup_i G_i$.

Example: Pseudospectral containment

Define $D = \{z : \|E(z)\| < \epsilon\}$. Then

1. $\Lambda(A + E) \subset \Lambda_\epsilon(A) \cup D^C$
2. A bounded component of $\Lambda_\epsilon(A)$ strictly inside D contains the same number of eigs of A and $A + E$.

Application: Lattice Schrödinger

Consider the discrete analogue to Schrödinger's equation:

$$H\psi = (-T + V)\psi = E\psi$$

where

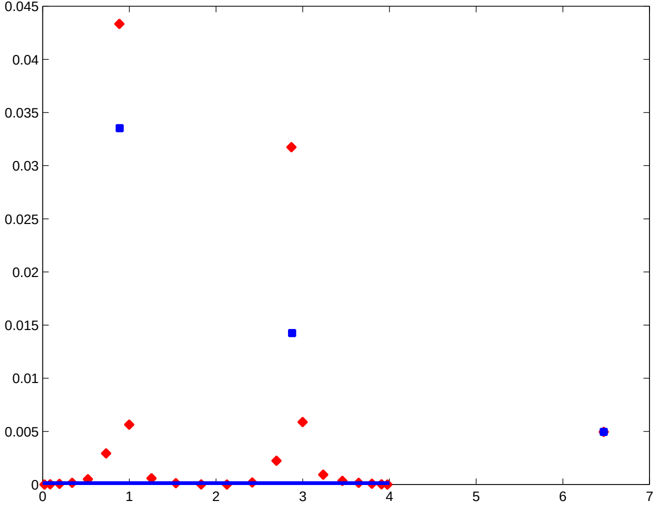
$$(H\psi)_k = -\psi_{k-1} + 2\psi_k - \psi_{k+1} + V_k\psi_k.$$

Assume $V_k = 0$ for $k \leq 0$ and $k \geq L$. May be complex.

Want to relate the spectrum for two variants:

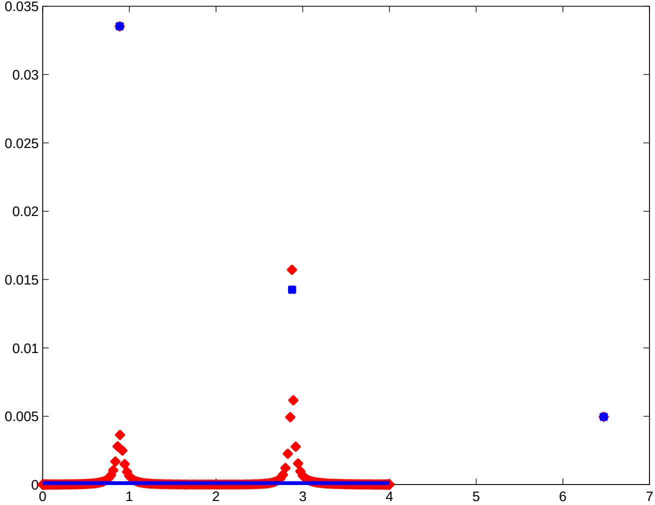
1. Non-negative integers: $\psi_0 = 0$ and $\psi \in l^2$
2. Bounded: $\psi_k = 0$ for $k = 0$ and $k \geq L + N$.

Application: Lattice Schrödinger



For $V_1 = 0.1i$ and $V_2 = 4$, $N = 20$.

Application: Lattice Schrödinger



For $V_1 = 0.1i$ and $V_2 = 4$, $N = 200$.

Spectral Schur Complement

Write H in either case as

$$H = \begin{bmatrix} -T_{11} + V_{11} & -e_L e_1^T \\ -e_L e_1^T & -T_{22} \end{bmatrix}$$

Then $\Lambda(H) \cap \Lambda(-T_{22})^c = \Lambda(S)$, where

$$S(z) = (-T_{11} + V_{11}) - zI - \left(e_1^T (-T_{22} - zI)^{-1} e_1 \right) e_L e_L^T$$

Write $S^{(N)}(z)$ and $S^{(\infty)}(z)$ for bounded and unbounded cases.

Spectral Schur Complement

For $z \notin [0,4]$, choose $\xi^2 - (2-z)\xi + 1 = 0$, $|\xi| < 1$. Then

$$\begin{aligned} S^{(\infty)}(z) &= (-T_{11} + V_{11}) - zI - \xi e_L e_L^T \\ S^{(N)}(z) &= (-T_{11} + V_{11}) - zI - \xi \left(\frac{1 - \xi^{2N}}{1 - \xi^{2(N+1)}} \right) e_L e_L^T \end{aligned}$$

Convenient to write $z = 2 - \xi - \xi^{-1}$, use ξ as primary variable.

Error Bounds

Find $\|S^{(\infty)} - S^{(N)}\| \leq \epsilon$ if

$$|\xi| < \left(1 + \frac{\log(3\epsilon^{-1})}{2N+1}\right)^{-1} = 1 - O\left(\frac{\log(\epsilon^{-1})}{N}\right).$$

Therefore, eigenvalues in bounded case (in ξ plane) either

1. Are within $O(\log(\epsilon^{-1})/N)$ of circle (continuous spectrum)
2. Are in $\Lambda_\epsilon(S^{(\infty)})$.

Get exponential convergence to discrete spectrum, linear convergence to continuous spectrum.

Error Estimate

If $S^{(\infty)}$ has an isolated eigenvalue at γ, then $S^{(N)}$ asymptotically has eigenvalues $\gamma^{(N)} \to \gamma$ with

$$\gamma^{(N)} - \gamma = \gamma^{2N} \frac{w^* e_L e_L^T v_L}{(1-\gamma^2) w^* v - w^* e_L e_L^T v} + O(\gamma^{2N+1})$$

where $S^{(\infty)}(\gamma) v = 0$ and $w^* S^{(\infty)}(\gamma) = 0$.

Similar Applications

- Linear stability analysis for traveling waves.
- Bounds on distance to instability via subspace projections.
- Estimates of damping in MEMS resonators.

Conclusions

- Can write eigenvalue and resonance problems via NEP
- Variational characterization gives easy first-order perturbation theory
- For analytic NEPs, also get analogues to standard perturbation bounds (Rouché, Gerschgorin, pseudospectral)
- Get interesting problems via approximation of spectral Schur complements