Applications and Analysis of Nonlinear Eigenvalue Problems

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Consider
\[ y'(t) - Ay(t) = f(t), \quad y(0) = 0. \]

Laplace transform:
\[ (s - A)Y(s) = F(s). \]

Special homogeneous solutions \( y(t) = e^{\lambda t}v \) s.t.
\[ (A - \lambda I)v = 0. \]
Quadratic Problem

Damped system:

\[ M u''(t) + B u'(t) + K u(t) = f(t). \]

Fourier transform:

\[ (-\omega^2 M + i\omega B + K) U(\omega) = F(\omega) \]

Special homogeneous solutions \( u(t) = e^{i\omega t} v \) s.t.

\[ (-\omega^2 M + i\omega B + K) v = 0. \]
General Nonlinear Problem

System with delay

\[ u'(t) - Au(t) - Bu(t - \tau) = f(t). \]

Laplace transform

\[ (s - A - e^{-\tau s} B)U(s) = F(s). \]

Special homogeneous solutions \( u(t) = e^{\lambda t} v \) s.t.

\[ (s - A - e^{-\tau s} B)v = 0. \]
General Picture

Special solutions to differential equation

$\iff$

Singularities of transformed system

$\iff$

Solutions to $A(\lambda)v = 0$, $A : \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$ meromorphic
Consider 1D Schrödinger ($V$ nice, $\text{supp}(V) \subset [a, b]$):

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

Restrict to domain $(a, b)$:

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

$$\left( \frac{d}{dx} + \sqrt{-E} \right) \psi = 0, \quad x = b$$

$$\left( \frac{d}{dx} - \sqrt{-E} \right) \psi = 0, \quad x = a$$

NEP with branch cut! Let’s change variables...
1D Schrödinger

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

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

Restrict to domain $(a, b)$, $E = k^2$:

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

$$\left(\frac{d}{dx} - ik\right)\psi = 0, \quad x = b$$

$$\left(\frac{d}{dx} + ik\right)\psi = 0, \quad x = a$$

$\text{Im} \ k \geq 0$ for eigenvalues, $\text{Im} \ k < 0$ for resonances.
Consider real $k > 0$, $\psi_0 = e^{ikx}$:

$$\left(-\frac{d^2}{dx^2} + V(x) - k^2\right)(\psi_0 + \psi_{\text{scatter}}) = 0, \quad x \in (a, b)$$

$$\left(\frac{d}{dx} - ik\right)\psi_{\text{scatter}} = 0, \quad x = b$$

$$\left(\frac{d}{dx} + ik\right)\psi_{\text{scatter}} = 0, \quad x = a$$

Define *transmission* $T(E) = T(k^2) = |\psi_{\text{scatter}}(b)|^2$. What happens to transmission near a resonance?
Resonances and Transmission

\[
\left(-\frac{d^2}{dx^2} + V(x) \right) \psi = 0, \quad V(x) = 5 \chi_{[0,L]}(x).
\]
Pseudospectral collocation at Chebyshev points:

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

\[
(D - ik) \psi = 0, \quad x = b
\]

\[
(D + ik) \psi = 0, \quad x = a
\]

Convert to linear problem with auxiliary variable \( \phi = k\psi \).
Is it that easy?
Is it that easy?

Potential

Pole locations
Backward Error Analysis

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

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

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.
$\lambda$ a simple eigenvalue of $A$, $w^*$ and $v$ eigenvectors. Formally differentiate $(A - \lambda)v = 0$:

$$(\delta A - \delta \lambda)v + (A - \lambda)\delta v = 0.$$ 

Multiply by $w^*$:

$$w^*(\delta A - \delta \lambda)v = 0.$$ 

Perturbation formula:

$$\delta \lambda = \frac{w^*(\delta A)v}{w^*v}.$$
If $\hat{w} = w + O(\epsilon)$, $\hat{v} = v + O(\epsilon)$,

$$\lambda = \frac{\hat{w}^* A \hat{v}}{\hat{w}^* \hat{v}} + O(\epsilon^2)$$

If $A$ is Hermitian, know $w^* = v^*$; gives

$$\lambda = \frac{\hat{v}^* A \hat{v}}{\hat{v}^* \hat{v}} + O(\epsilon^2)$$

so eigenvalues are stationary points of Rayleigh quotient

$$\rho_A(x) = \frac{x^* A x}{x^* x}.$$
Consider simple eigenvalue for $A : \mathbb{C} \to \mathbb{C}^{n \times n}$.
Formally differentiate $A(\lambda)v = 0$ and multiply by $w$ to get

$$\delta \lambda = \frac{w^*(\delta A(\lambda))v}{w^*A'(\lambda)v}.$$ 

If $A$ always Hermitian, implicitly define functional $\rho_A(x)$ by

$$x^*A(\rho_A(x))x = 0.$$ 

Stationary points for $\rho_A(x)$ correspond to eigenvalues.
Similar trick works for $A$ symmetric.
Variational Formulation for Scattering

Consider Schrödinger with compactly supported $V$ in $R^d$. Seek

$$(H_V - k^2)\psi = f \text{ on } \Omega$$

$$\frac{\partial \psi}{\partial n} - B(k)\psi = 0 \text{ on } \Gamma$$

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

$$I(\psi) = \frac{1}{2} \int_{\Omega} \left( (\nabla \psi)^T (\nabla \psi) + \psi (V - k^2) \psi \right) \, d\Omega + \frac{1}{2} \int_{\Gamma} \psi B(k) \psi \, d\Gamma - \int_{\Omega} \psi f \, d\Omega.$$
Check variational formulation:

\[ I(\psi) = \frac{1}{2} \int_{\Omega} \left( (\nabla \psi)^T (\nabla \psi) + \psi (V - k^2) \psi \right) \, d\Omega - \frac{1}{2} \int_{\Gamma} \psi B(k) \psi \, d\Gamma - \int_{\Omega} \psi f \, d\Omega. \]

Use symmetry of form (note \( \int_{\Gamma} \phi B(k) \psi = \int_{\Gamma} \psi B(k) \phi \)) + integration by parts:

\[ \delta I(\psi) = \int_{\Omega} \delta \psi \left( -\Delta \psi + (V - k^2) \psi - f \right) \, d\Omega + \int_{\Gamma} \delta \psi \left( \frac{\partial \psi}{\partial n} - B(k) \right) \psi \, d\Gamma. \]
Variational Formulation for Resonances

Now define a residual for an approximate eigenpair:

\[ r(\psi, k) = \int_{\Omega} \left( (\nabla \psi)^T (\nabla \psi) + \psi (V - k^2) \psi \right) - \int_{\Gamma} \psi B(k) \psi. \]

Take variations and use symmetry of \( B \):

\[
\delta r(\psi, k) = 2 \int_{\Omega} \delta \psi \left[ (-\Delta + V - k^2) \psi \right] + \\
2 \int_{\Gamma} \delta \psi \left[ \frac{\partial \psi}{\partial n} - B(k) \psi \right] + \\
\delta k \left[ 2k \int_{\Omega} \psi^2 - \int_{\Gamma} \psi B'(k) \psi \right]
\]

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

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

Stationary precisely when $(\psi, k)$ an eigenpair.
Sensitivity

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

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

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

$$
\delta k = \frac{\int_{\Omega} \psi (-\Delta + (V + \delta V) - k^2) \psi}{2k \int_{\Omega} \psi^2 - \int_{\Gamma} \psi B'(k) \psi}.
$$
1. Compute approximate solution \((\hat{\psi}, \hat{k})\).

2. Map \(\hat{\psi}\) to high-resolution quadrature grid to evaluate

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

3. If \(\delta k\) large, discard \(\hat{k}\) as spurious; otherwise, accept \(k \approx \hat{k} + \delta k\).
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.
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

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

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

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

\[
\Sigma(x) = \int_0^x \sigma(s) \, ds
\]
Model with Perfectly Matched Layer

If solution clamped at $x = L$ then

$$\frac{C_{in}}{C_{out}} = O(e^{-k\gamma}) \text{ where } \gamma = \Sigma(L) = \int_{0}^{L} \sigma(s) \, ds$$
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

$\Re(\tilde{x})$

$\Re(\tilde{x})$
Model Problem Illustrated

Outgoing \(\exp(-ix)\) 
Incoming \(\exp(ix)\)

Transformed coordinate

\(\text{Re}(\tilde{x})\)
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$  
Incoming $\exp(i\tilde{x})$

Transformed coordinate

Re($\tilde{x}$)

$0 2 4 6 8 10 12 14 16 18$

$0 5 10 15 20$

$-4 -2 0 2 4 6$

$-1 -0.5 0 0.5 1$
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

$\Re(\tilde{x})$
Model Problem Illustrated

\[ \text{Outgoing exp}(−i\tilde{x}) \quad \text{Incoming exp}(i\tilde{x}) \]

\[ \text{Transformed coordinate} \]

\[ \text{Re}(\tilde{x}) \]

\[ 0 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10 \quad 12 \quad 14 \quad 16 \quad 18 \]

\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \]

\[ -4 \quad -2 \quad 0 \quad 20 \quad 40 \]

\[ -1 \quad -0.5 \quad 0 \quad 0.5 \quad 1 \]
Model Problem Illustrated

Outgoing \(\exp(-i\tilde{x})\)  

Incoming \(\exp(i\tilde{x})\)

Transformed coordinate

\(\text{Re}(\tilde{x})\)
Finite/Spectral Element Implementation

Combine PML and isoparametric mappings

\[ k_{ij}^e = \int_{\Omega} (\tilde{\nabla} N_i)^T D (\tilde{\nabla} N_j) \tilde{J} \, d\Omega \]

\[ m_{ij}^e = \int_{\Omega} \rho N_i N_j \tilde{J} \, d\Omega \]

- Matrices are \textit{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 $\implies$ 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?
General NEP Picture

\[ A : \mathbb{C} \rightarrow \mathbb{C}^{n \times n} \text{ analytic in } \Omega \]

\[ \Lambda(A) := \{ z \in \mathbb{C} : A(z) \text{ singular} \} \]

\[ \Lambda_{\epsilon}(A) := \{ z \in \mathbb{C} : \| A(z)^{-1} \| \geq \epsilon^{-1} \} \]

- 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 $\Gamma$, analytic inside, count eigs inside by

$$W_\Gamma(\det(A)) = \frac{1}{2\pi i} \int_\Gamma \frac{d}{dz} \ln \det(A(z)) \, dz$$

$$= \text{tr} \left( \frac{1}{2\pi i} \int_\Gamma A(z)^{-1} A'(z) \, dz \right)$$

Suppose $E$ also analytic inside $\Gamma$. By continuity,

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

for $s$ in neighborhood of $0$ such that $A + sE$ remains nonsingular on $\Gamma$. 
Winding number counts give continuity of eigenvalues $\Rightarrow$
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

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

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

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

Proof: Write \( A = D + F \) where \( D = \text{diag}(A) \). \( D + sF \) is diagonally dominant (so invertible) off \( \bigcup_i G_i \).
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 $A + E$. 
Other Applications

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

▶ Nonlinear eigenproblems tell us interesting information about dynamics.
▶ Analytic structure of the eigenproblem is key to error analysis.
▶ Variational characterization gives easy first-order perturbation theory
▶ Also get analogues to standard perturbation bounds (Rouché, Gerschgorin, pseudospectral)
▶ Get interesting estimates via approximation of spectral Schur complements