Applications and Analysis of Nonlinear Eigenvalue Problems

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Linear Problem

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:

$$Mu''(t) + Bu'(t) + Ku(t) = f(t).$$

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

$\Longleftrightarrow$

Singularities of transformed system

$\Longleftrightarrow$

Solutions to $A(\lambda)v = 0$, $A : \mathbb{C} \to \mathbb{C}^{n\times n}$ meromorphic

1D Schrödinger

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

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

Restrict to domain (a, b):

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

NEP with branch cut! Let's change variables...

1D Schrödinger

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

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

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

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

Im $k \geq 0$ for eigenvalues, Im $k < 0$ for *resonances*.

1D Schrödinger scattering

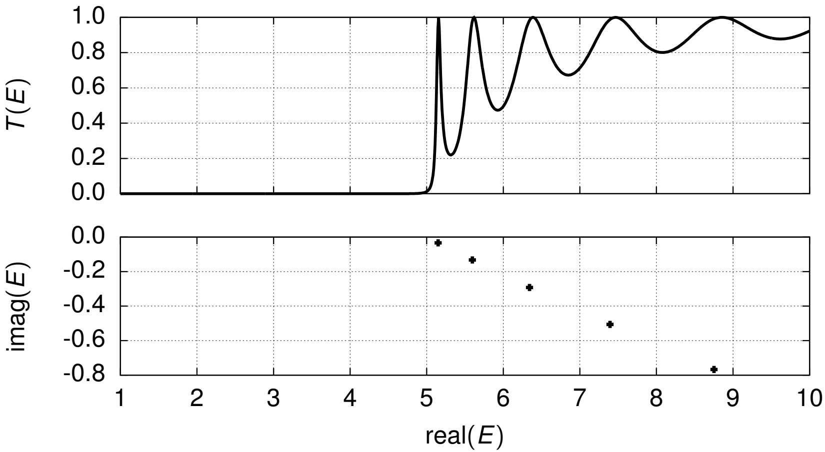
Consider real $k > 0$, $\psi_0 = e^{ikx}$:

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

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

Resonances and Transmission

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = 0, \qquad V(x) = 5\,\chi_{[0,L]}(x).$$



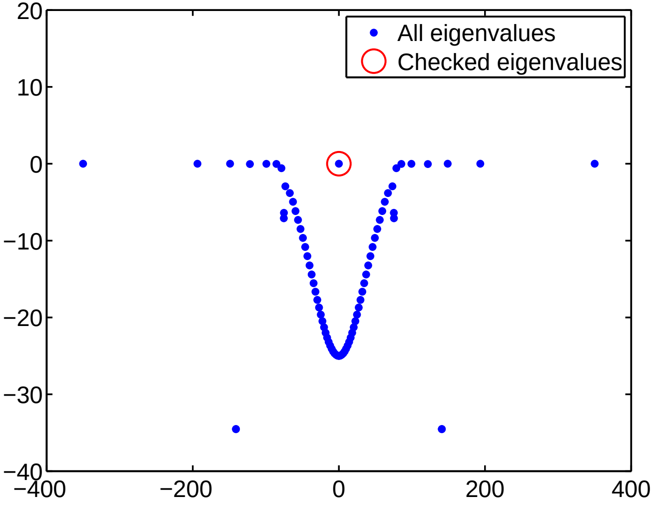
Computing Resonances

Pseudospectral collocation at Chebyshev points:

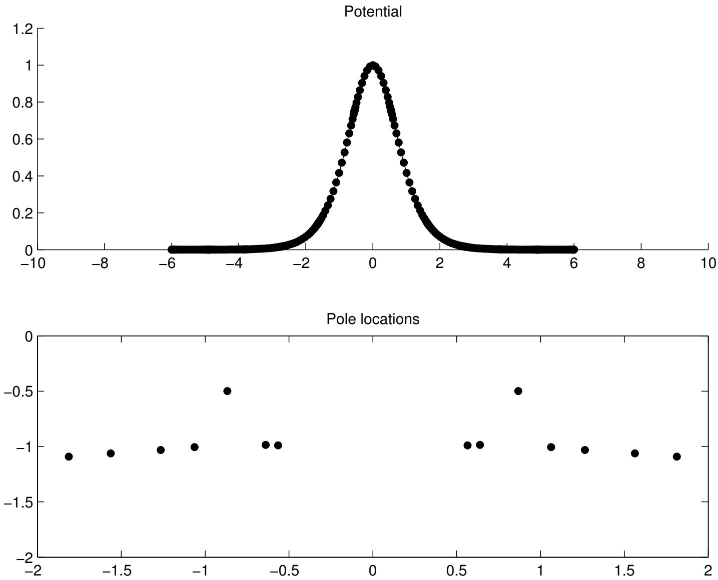
$$\begin{aligned} \left(-D^2 + V(x) - k^2\right)\psi &= 0, \quad x \in (a, b) \\ (D - ik)\,\psi &= 0, \quad x = b \\ (D + ik)\,\psi &= 0, \quad x = a \end{aligned}$$

Convert to linear problem with auxiliary variable $\phi = k\psi$.

Is it that easy?



Is it that easy?



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.

Reminder: Eigenvalue Perturbations

λ 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:

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

Rayleigh Quotients

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

$$\rho_A(x) = \frac{x^* A x}{x^* x}.$$

Transition to NEPs

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

$$
\begin{aligned}
(H_V - k^2)\psi &= f \text{ on } \Omega \\
\frac{\partial \psi}{\partial n} - B(k)\psi &= 0 \text{ on } \Gamma
\end{aligned}
$$

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

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

Variational Formulation for Scattering

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:

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

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

Rayleigh Quotient Analogue

We now implicitly define a differentiable function $\tilde{k}(\phi)$ in the neighborhood of an eigenpair (ψ, 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 (ψ, k) 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

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

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

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

Backward Error Analysis Revisited

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 δk 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.

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

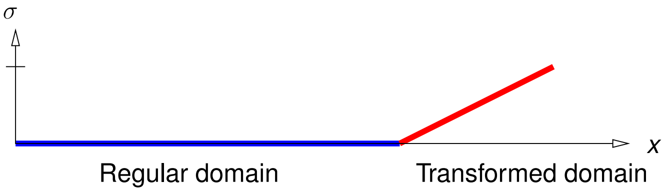
- Domain: $x \in [0, \infty)$
- Frequency-domain equation:

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

- Solution:

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

Model with Perfectly Matched Layer

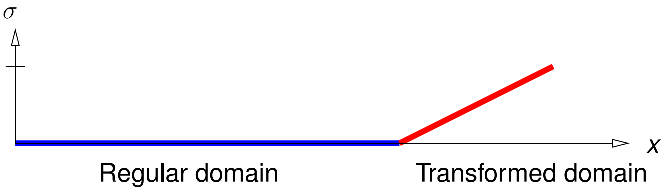


$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

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

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

Model with Perfectly Matched Layer



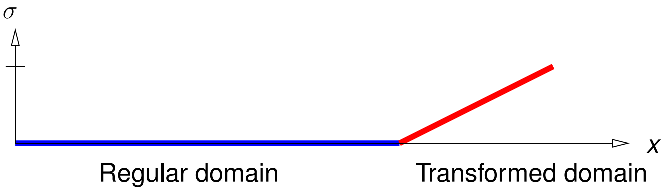
$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

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

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

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

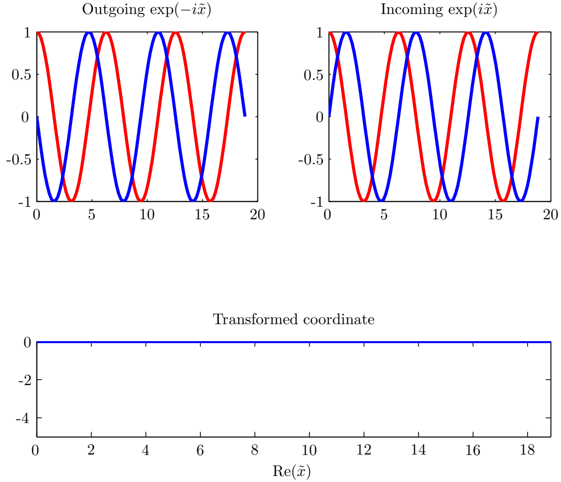
Model with Perfectly Matched Layer



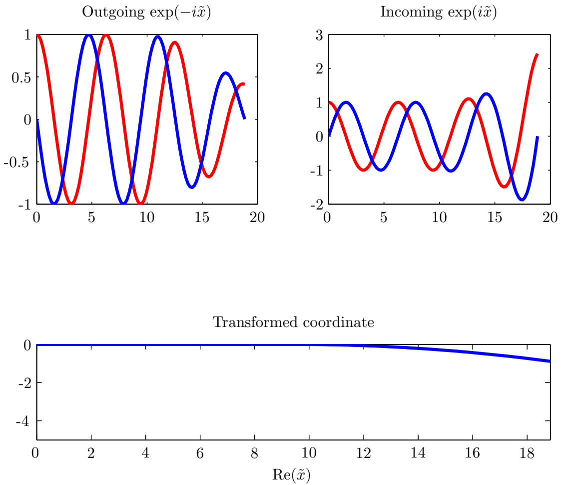
If solution clamped at $x = L$ then

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

Model Problem Illustrated



Model Problem Illustrated



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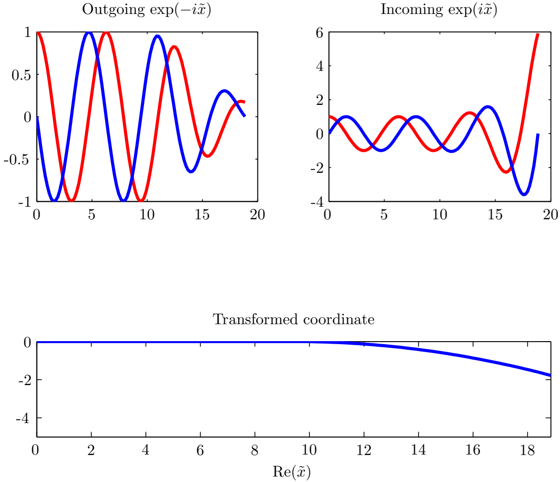
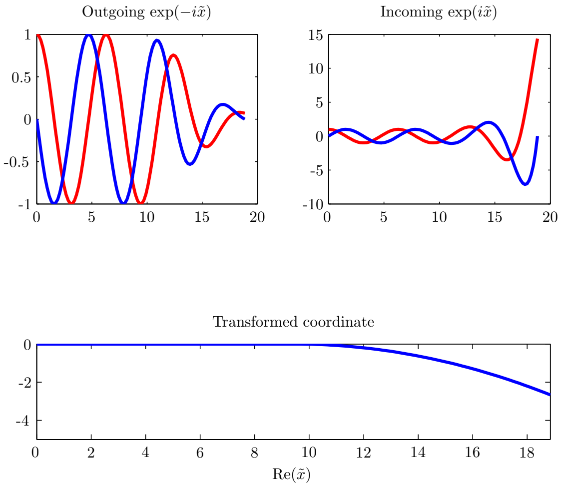
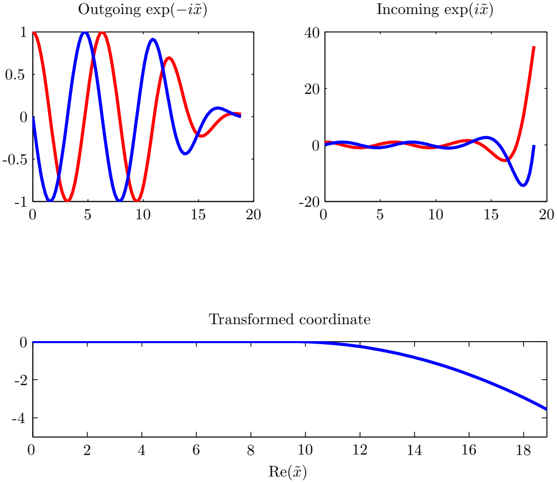


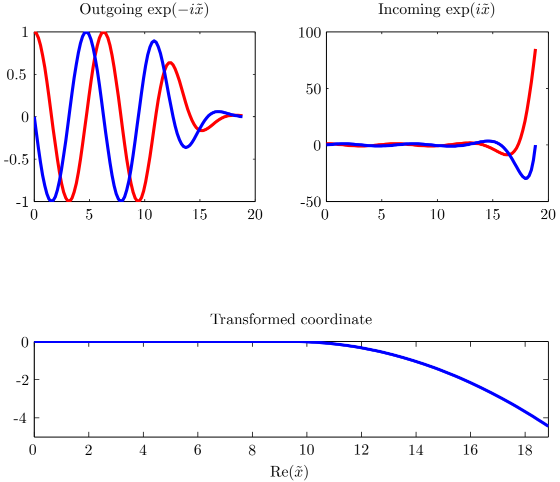
Model Problem Illustrated



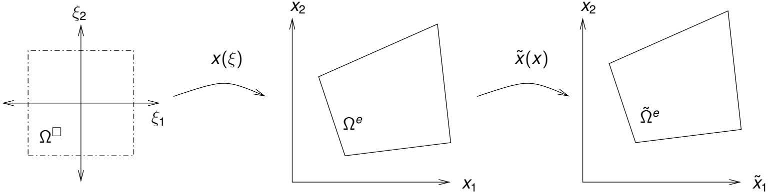
Model Problem Illustrated



Model Problem Illustrated



Finite/Spectral Element Implementation



- Combine PML and isoparametric mappings

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

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

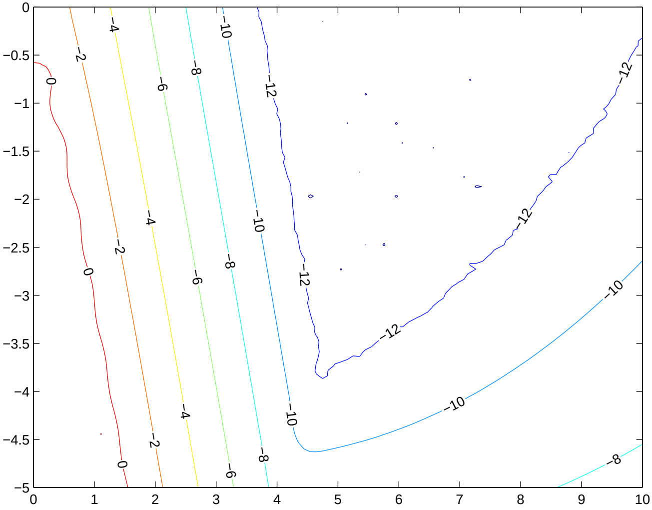
- Matrices are *complex symmetric*

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.

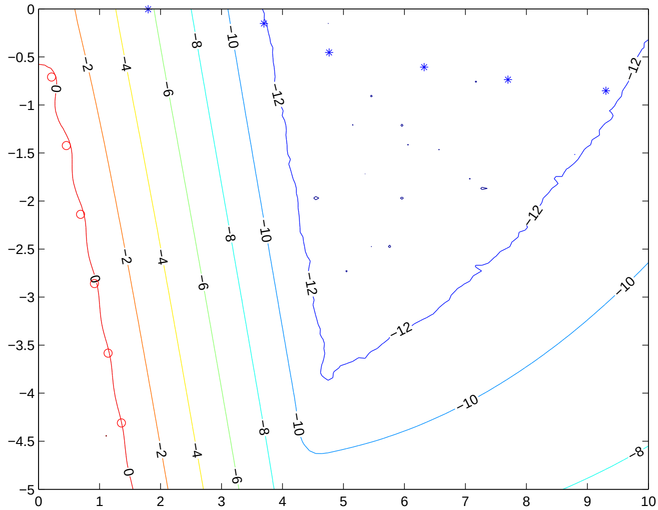
DtN Approximation in PML

$\log_{10} |B(k)_{PML} - B(k)|$ 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?

General NEP Picture

$A : \mathbb{C} \to \mathbb{C}^{n \times n}$ 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 $\implies$
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 $A + E$.

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