Numerical Analysis of Resonances

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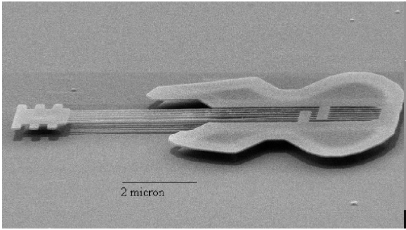
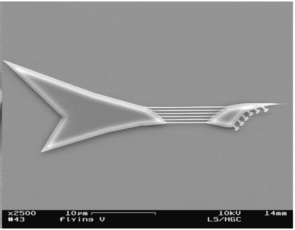
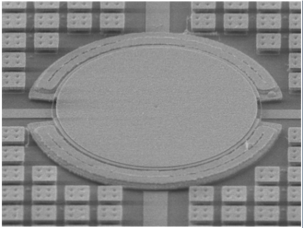
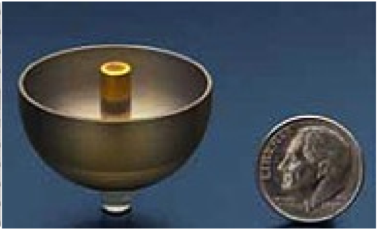
My favorite applications

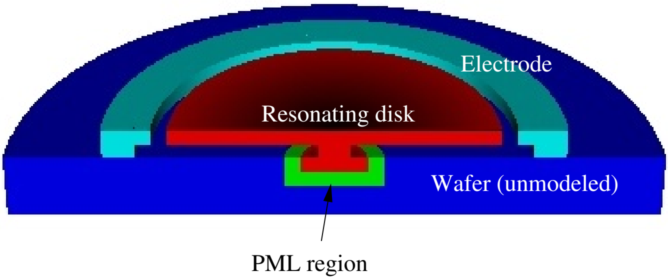




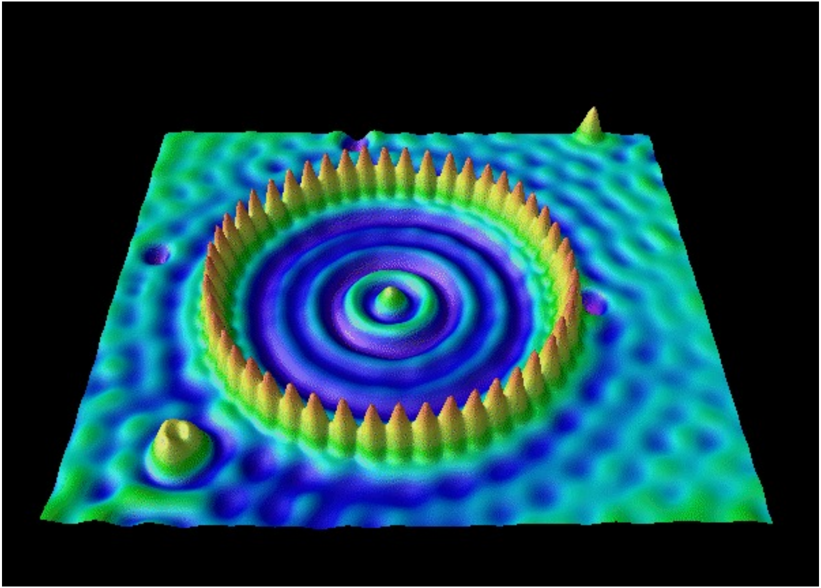




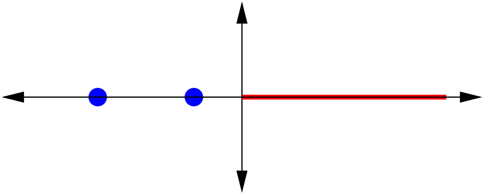
Resonance and anchor loss



The quantum corral and tunneling

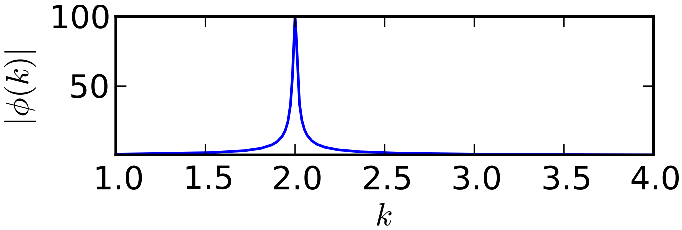


Spectra and scattering



Spectrum for $H = -\Delta + V$, $\mathrm{supp}(V)$ compact.

Resonances and scattering



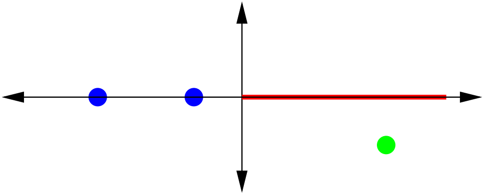
For $\text{supp}(V) \subset \Omega$, consider a scattering experiment:

$$(H - k^2)\psi = f \text{ on } \Omega$$
$$(\partial_n - B(k))\psi = 0 \text{ on } \partial\Omega$$

See resonance peaks (Breit-Wigner):

$$\phi(k) \equiv w^* \psi \approx C(k - k^*)^{-1}.$$

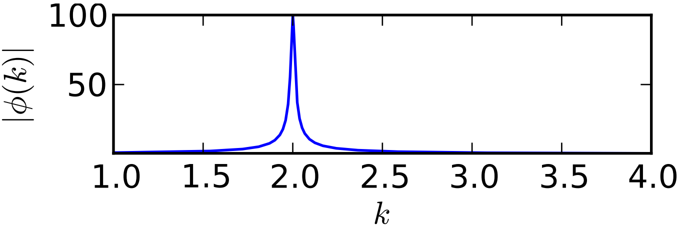
Resonances and scattering



Consider a scattering measurement $\phi(k)$

- Morally looks like $\phi = w^*(H-E)^{-1}f$?
- $w^*(H-E)^{-1}f$ is well-defined off spectrum of H
- Continuous spectrum of H is a branch cut for ϕ
- Resonance poles are on a *second sheet of definition* for ϕ
- Resonance “wave functions” blow up exponentially (not L^2)

Common approach



Goal: Understand localized “leaky” vibrations

- Far field $\approx$ infinite and homogeneous
- Dynamics $\approx$ truncated resonance expansion (Breit-Wigner):

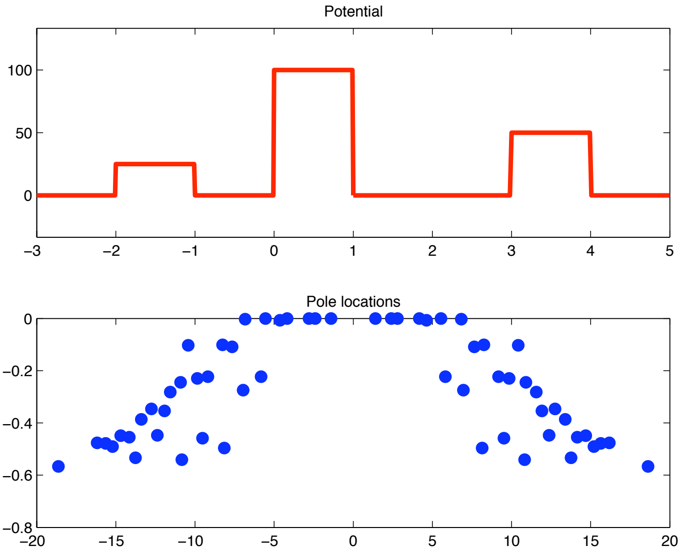
$$\phi(k) \approx C(k - k^*)^{-1}, \quad k_* \in \mathbb{C}$$

Reduce to a bounded domain and compute!

The 1D case: MatScat

http://www.cs.cornell.edu/~bindel/cims/matscat/

MatScat



Potential
100
50
0
–3
–2
–1
0
1
2
3
4
5
Pole locations
0
–0.2
–0.4
–0.6
–0.8
–20
–15
–10
–5
0
5
10
15
20

Resonances and transients

(Loading outs.mp4)

Scattering solutions

Schrödinger scattering from a potential V on $[a, b]$

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

For $E = k^2 > 0$, get solutions

$$\psi = e^{-ikx} + \psi_{\text{scatter}}$$

where ψ_{scatter} satisfies outgoing BCs:

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

This is a *Dirichlet-to-Neumann* (DtN) map: $(\partial_n - B(k))\psi = 0$

A quadratic eigenvalue problem

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

Look for nontrivial solutions:

- $\mathrm{Im}(k) > 0$: Bound states
- $\mathrm{Im}(k) < 0$: Resonances

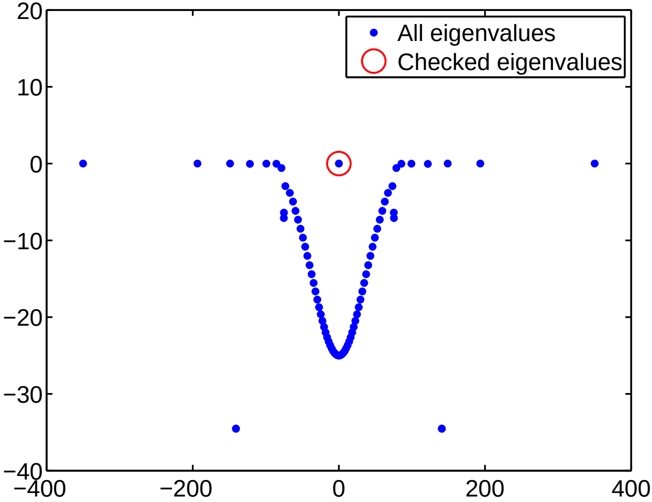
Basic MatScat strategy

Pseudospectral collocation at Chebyshev points:

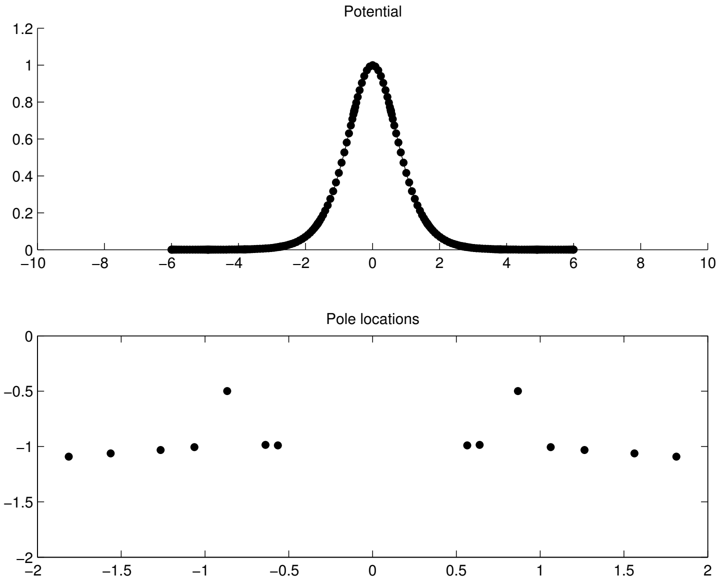
$$\begin{aligned}\left(-D^2 + V(x) - k^2\right)\psi &= 0, \quad x \in (a,b)\\ (D - ik)\,\psi &= 0, \quad x = b\\ (D + ik)\,\psi &= 0, \quad x = a\end{aligned}$$

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

Is it that easy?



Is it that easy?



Computational desiderata

- All resonances in some region
- *and* error estimates
- *and* sensitivity estimates
- *and* good computational complexity

Method 1: Prony and company

Extract resonances from time-domain data (or $\phi(k)$)

$$u(t) \approx \sum_k c_k \exp(\lambda_k t)$$

- This is a (modified) *Prony* problem
- Long use both experimentally and computationally (e.g. Wei-Majda-Strauss, JCP 1988 – modified Prony applied to time-domain simulations)
- Variants like FDM still used (e.g. Johnson's `harminv`)

Computing resonances 2: complex scaling

Change coordinates to shift the branch cut:

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

where $d\hat{x}/dx = 1 + i\sigma(x)$ is deformed outside $[a, b]$.

- Rotates the continuous spectrum to reveal resonances
- First used to *define* resonances (Simon 1979)
- Also a computational method (aka PML):
  - Truncate to a finite $\tilde{x}$ domain.
  - Discretize using standard methods
  - Solve a complex symmetric eigenvalue problem

One of my favorite computational tactics.

Computing resonances 3: a nonlinear eigenproblem

Can also define resonances via a NEP:

$$(H - k^2)\psi = 0 \text{ on } \Omega$$
$$(\partial_n - B(k))\psi = 0 \text{ on } \partial\Omega$$

Resonance solutions are stationary points with respect to ψ of

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

Discretized equations (e.g. via finite or spectral elements) are

$$A(k)\psi = \left(K - k^2 M - C(k) \right) \psi = 0$$

K and M are real symmetric and $C(k)$ is *complex* symmetric.

Computational tradeoffs

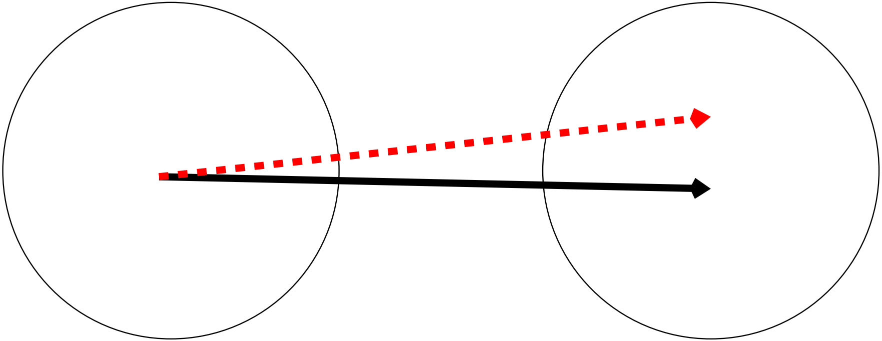
- Prony
  - Relatively simple signal processing
  - Can be used with scattering experiment results
  - May require long simulations
  - Numerically sensitive
- Complex scaling
  - Straightforward implementation
  - Yields a *linear* eigenvalue problem
  - How to choose scaling parameters, truncation?
- DtN map formulation
  - Bounded domain — no artificial truncation
  - Yields a *nonlinear* eigenvalue problem
  - DtN map is spatially nonlocal except in 1D (though diagonalized by Fourier modes on a circle)

Other options: complex absorbing potentials, approximate BCs (e.g. Engquist-Majda)

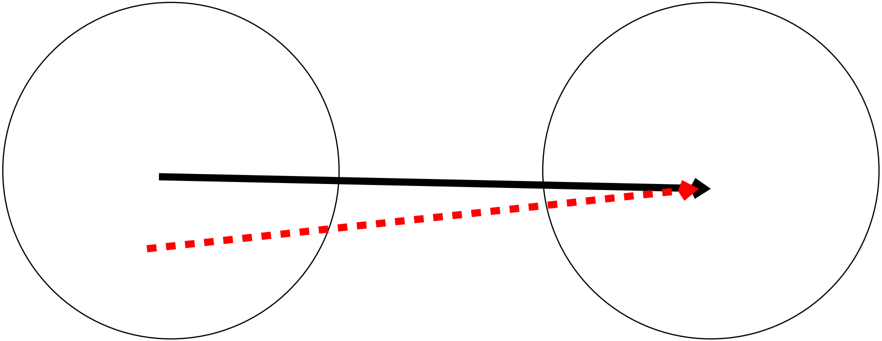
Computational desiderata

- All resonances in some region
- *and* error estimates
- *and* sensitivity estimates
- *and* good computational complexity

Forward and backward error analysis



Forward and backward error analysis



A simple example

Standard eigenvalue problem $(A - \lambda I)v = 0$, $\|v\| = 1$:

$$(A - \tilde{\lambda} I)\tilde{v} = r$$
$$(\tilde{A} - \tilde{\lambda} I)\tilde{v} = 0, \quad \tilde{A} = A - rv^T$$

So $\tilde{\lambda} \in \Lambda_\epsilon(A)$ and $\lambda \in \Lambda_\epsilon(\tilde{A})$, where $\Lambda_\epsilon(A) \equiv \{\|A^{-1}\| > \epsilon^{-1}\}$.

Or estimate $\tilde{\lambda} - \lambda$ by first-order sensitivity analysis

Sensitivity for resonances

Resonance solutions are stationary points with respect to ψ of

$$\Phi(\psi, k) = \int_\Omega \psi \left[-\nabla^2\psi + (V - k^2)\psi\right] d\Omega - \int_{\partial\Omega} \psi \left(\frac{\partial\psi}{\partial n} - B(k)\psi\right) d\Gamma$$

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

If (ψ, k) a resonance pair, then $\Phi(\psi, k) = 0$ and $D_\psi\Phi(\psi, k) = 0$.

Potential perturbations

If (ψ, k) a resonance pair, then $\Phi(\psi, k) = 0$ and $D_\psi \Phi(\psi, k) = 0$.

Consider perturbed V:

$$\delta\Phi = D_\psi \Phi \cdot \delta\psi + D_V \Phi \cdot \delta V + D_k \Phi \cdot \delta k = 0$$

Use $D_\psi \Phi \cdot \delta\psi = 0$:

$$\delta k = -\frac{D_V \Phi \cdot \delta V}{D_k \Phi}$$

Perturbation worked out

So look at how perturbations δV change k:

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

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 in MatScat

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 $\hat{k}$; otherwise, accept $k \approx \hat{k} + \delta k$.

Beyond 1D

1D was relatively easy:

- Only small discretizations needed.
- Worked with exact boundary conditions
- Could rewrite general NEP as a QEP

Nonlinear to linear eigenproblems

Can also compute resonances by

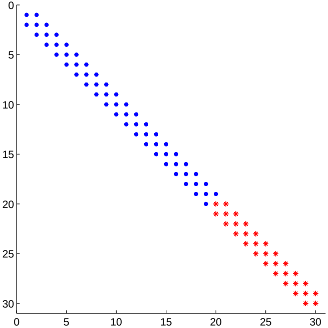
- Adding a complex absorbing potential
- Complex scaling methods
- Artificial dampers

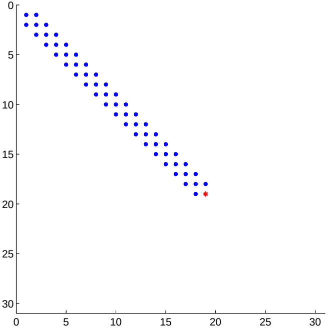
Both result in complex-symmetric ordinary eigenproblems:

$$(K_{ext} - k^2 M_{ext})\psi_{ext} = \left(\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} - k^2 \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = 0$$

where ψ_2 correspond to extra variables (outside Ω).

Spectral Schur complement





Eliminate “extra” variables ψ_2 to get

$$\hat{A}(k)\psi_1 = \left(K_{11} - k^2 M_{11} - \hat{C}(k)\right)\psi_1 = 0$$

where

$$\hat{C}(k) = (K_{12} - k^2 M_{12})(K_{22} - k^2 M_{22})^{-1}(K_{21} - k^2 M_{21})$$

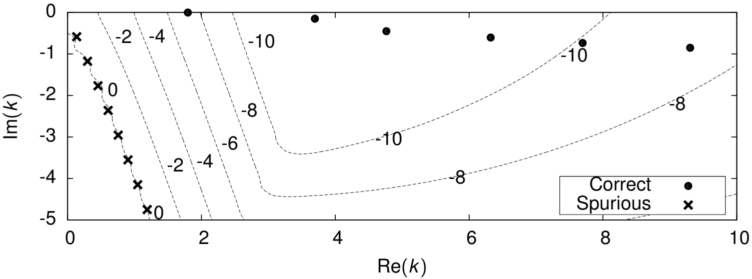
Apples to oranges?

$$A(k)\psi = (K - k^2 M - C(k))\psi = 0 \quad \text{(exact DtN map)}$$
$$\hat{A}(\hat{k})\hat{\psi} = (K - \hat{k}^2 M - \hat{C}(\hat{k}))\hat{\psi} = 0 \quad \text{(spectral Schur complement)}$$

Two ideas:

- Perturbation theory for NEP for local refinement
- Complex analysis to get more global analysis

Linear vs nonlinear



To get axisymmetric resonances in corral model, compute:

- Eigenvalues of a complex-scaled problem
- Residuals in nonlinear eigenproblem
- $\log_{10} \|A(k) - \hat{A}(k)\|$

Corrections two ways

$$A(k)\psi = (K - k^2 M - C(k))\psi = 0 \quad \text{(exact DtN map)}$$
$$\hat{A}(\hat{k})\hat{\psi} = (K - \hat{k}^2 M - \hat{C}(\hat{k}))\hat{\psi} = 0 \quad \text{(spectral Schur complement)}$$

- Plug $(\hat{k}, \hat{\psi})$ into true problem and correct:

$$k - \hat{k} \approx \frac{\hat{\psi}^T A(\hat{k})\hat{\psi}}{\hat{\psi}^T A'(\hat{k})\hat{\psi}}$$

- Write $A(k) = \hat{A}(k) + E(k)$ where $E(k) = C(k) - \hat{C}(k)$. Interpret $E(\hat{k})$ as a correction to K_{ext} in linear problem.

Latter is promising for analysis beyond first-order sensitivity.

A little complex analysis

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

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

$E = A - \hat{A}$ also analytic inside Γ. By continuity,

$$W_\Gamma(\det(A)) = W_\Gamma(\det(A+E)) = W_\Gamma(\det(\hat{A}))$$

if $A + sE$ nonsingular on Γ for $s \in [0, 1]$.

A general recipe

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

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

Application: Matrix Rouché

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

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

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

Aside on spectral Schur complement

Inverse of a Schur complement is a submatrix of an inverse:

$$(K_{ext} - z^2 M_{ext})^{-1} = \begin{bmatrix} \hat{A}(z)^{-1} & * \\ * & * \end{bmatrix}$$

So for reasonable norms,

$$\|\hat{A}(z)^{-1}\| \leq \|(K_{ext} - z^2 M_{ext})^{-1}\|.$$

Or

$$\Lambda_\epsilon(\hat{A}) \subset \Lambda_\epsilon(K_{ext}, M_{ext}),$$

$$\Lambda_\epsilon(\hat{A}) \equiv \{z : \|\hat{A}(z)^{-1}\| > \epsilon^{-1}\}$$
$$\Lambda_\epsilon(K_{ext}, M_{ext}) \equiv \{z : \|(K_{ext} - z^2 M_{ext})^{-1}\| > \epsilon^{-1}\}$$

Nonlinear bounds from linear pseudospectra

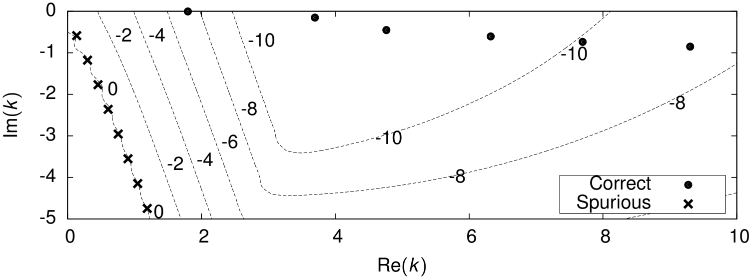
Recall:

$$A(k)\psi = (K - k^2 M - C(k))\psi = 0 \quad \text{(exact DtN map)}$$
$$\hat{A}(\hat{k})\hat{\psi} = (K - \hat{k}^2 M - \hat{C}(\hat{k}))\hat{\psi} = 0 \quad \text{(spectral Schur complement)}$$

Let $S_\epsilon = \{z \in \mathbb{C} : \|C(z) - \hat{C}(z)\| < \epsilon\}$. Then:

$$\Lambda(A) \cap S_\epsilon \subset \Lambda_\epsilon(\hat{A}) \subset \Lambda_\epsilon(K_{\mathrm{ext}}, M_{\mathrm{ext}})$$

Sensitivity and pseudospectra



Theorem

Let $S_\epsilon = \{z : \|A(z) - \hat{A}(z)\| < \epsilon\}$. Any connected component of $\Lambda_\epsilon(K_{ext}, M_{ext})$ strictly inside S_ϵ contains the same number of eigenvalues for $A(k)$ and $\hat{A}(k)$.

For more

More information at

`http://www.cs.cornell.edu/~bindel/`

- Links to tutorial notes on resonances with Maciej Zworski
- Matscat code for computing resonances for 1D problems
- These slides!