Computation and Continuation of Eigenvalues for Parameterized Nonlinear Eigenvalue Problems

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Based on joint work with
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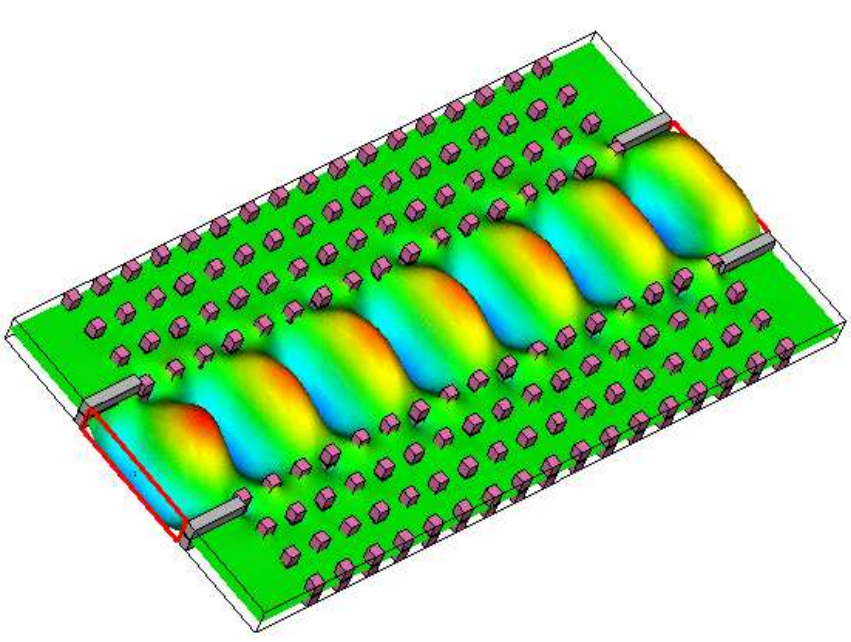
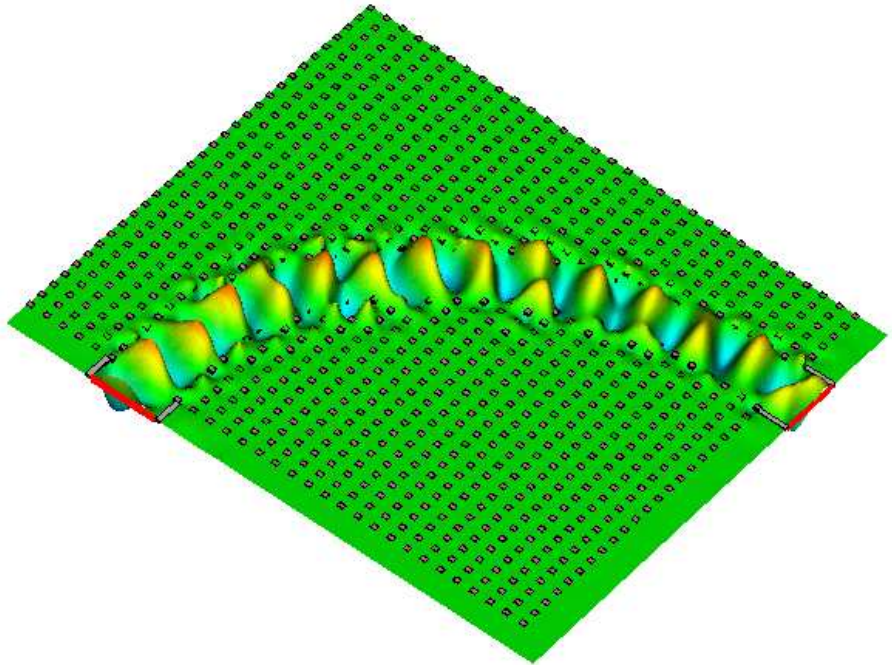
Outline

- Motivating application:
  Band structure calculation for photonic crystals
- Solution of rational eigenvalue problems by linearization
- Invariant pairs for nonlinear eigenvalue problems
- Detecting and augmenting non-simple invariant pairs

Motivating Application

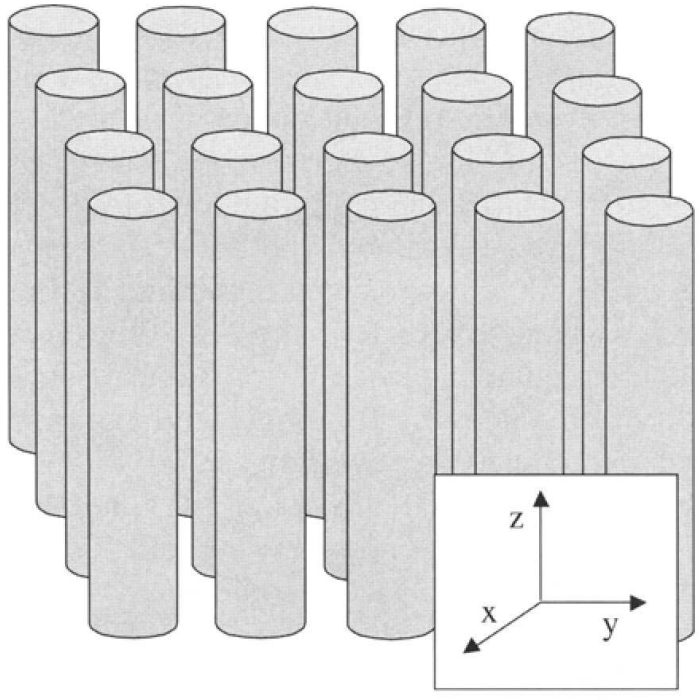
Photonic crystals





- photonic crystal = lattice of mixed dielectric media
- control light by designing media that prohibits propagation of electromagnetic waves in certain frequency range
- complete photonic band gap = frequency range with no propagation of electromagnetic waves of *any* polarization travelling in *any* direction.
- Freely available online: *Photonic Crystals: Molding the Flow of Light, 2nd ed., J. D. Joannopoulos et al., Princeton University Press, 2008.*

2D periodic crystal



- material periodic along x- and y-direction; homogeneous along z-direction
- consider only electromagnetic waves with propagation in xy-plane

Mathematical model

Time-harmonic modes of electromagnetic wave (E, H) (E electric field, H magnetic field) decompose:

- transverse electric (TE) polarized modes $(E_x, E_y, 0, 0, 0, H_z)$
- transverse magnetic (TM) polarized modes $(0, 0, E_z, H_x, H_y, 0)$

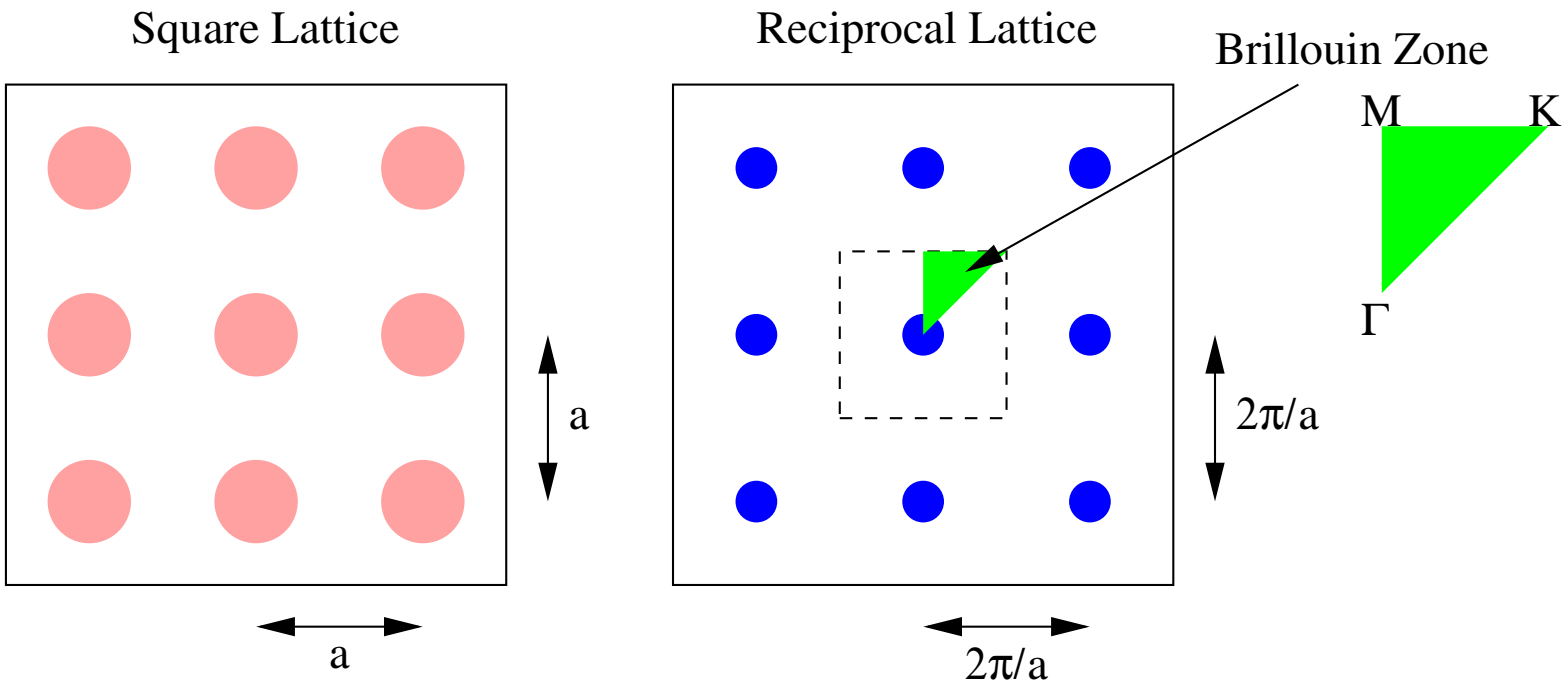
Macroscopic Maxwell equations $\rightsquigarrow$ scalar equation for E_z of TM-mode at frequency ω:

$$-\Delta E_z = \omega^2 \epsilon(r, \omega) E_z,$$

where $r = (x, y)$ and ϵ denotes relative permittivity.

Material parameter $\epsilon(r, \omega)$ usually depends on the frequency of the time-harmonic wave!

Bloch solutions



By Bloch's theorem, E_z takes the form

$$E_z(r) = e^{ik\cdot r}u(r),$$

where k is a wave vector $\in$ Brillouin zone, $u(r)$ periodic on lattice $\rightsquigarrow$

$$-(\nabla + ik)\cdot(\nabla + ik)u(r) = \omega^2\epsilon(r,\omega)u(r)$$

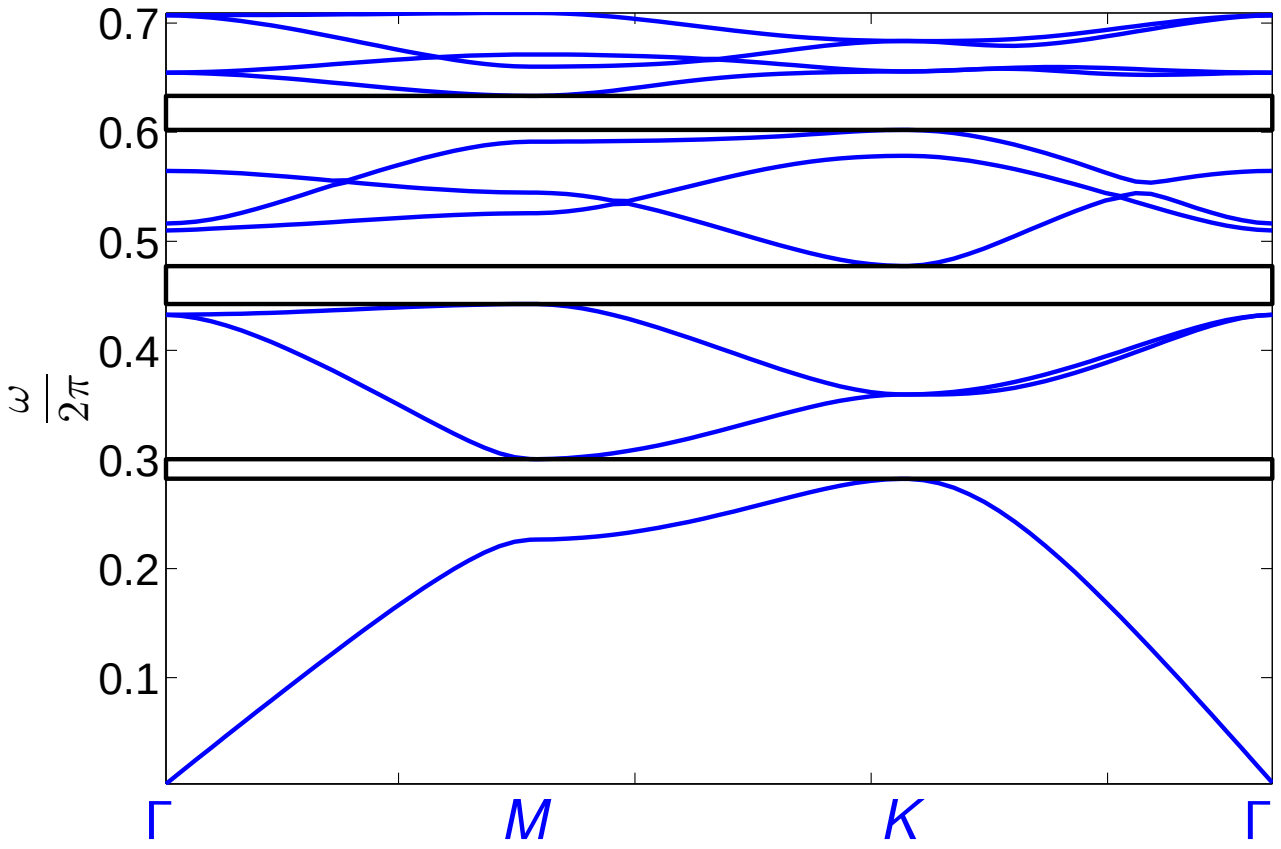
Finding band gaps

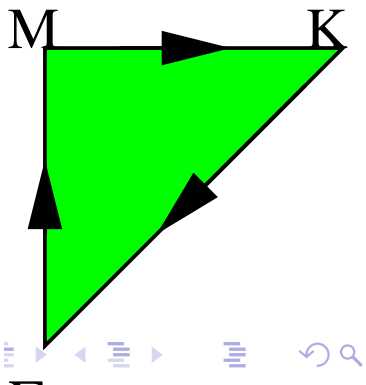
Goal: Find frequency ranges $[\omega_{\text{low}}, \omega_{\text{high}}]$ for which

$$-(\nabla + \mathrm{i}k) \cdot (\nabla + \mathrm{i}k)u(r) = \omega^2 \epsilon(r, \omega) u(r)$$

has *no* solution.

Band structure diagram:





Finding band gaps

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has *no* solution.

Assuming two different materials, finite element discretization $\rightsquigarrow$

$$\big(G(k) - \omega^2 \epsilon_1(\omega) M_1 - \omega^2 \epsilon_2(\omega) M_2\big) x = 0, \quad x \neq 0.$$

with M_1, M_2 symm pos semidef, $G(k)$ Herm pos def.

- Eigenvalue problem nonlinear in eigenvalue parameter ω.
- Nonlinearity due to frequency-dependent permittivity $\epsilon_j(\omega)$.
- 2D problem on uncomplicated domains $\rightsquigarrow$ excellent accuracy for $n = O(10^4)$ using high-order FEs.

Lorentz permittivity model

Example: $\epsilon_1 \equiv 1$ and $\epsilon_2(\omega)$ models observed material properties.

- Popular: Lorentz permittivity model

$$\epsilon_2(\omega) = \alpha + \sum_{k=1}^{K} \frac{\xi_k}{\eta_k - \omega^2 - \mathbf{i}\gamma_k\omega},$$

with parameters $\alpha, \xi_k, \eta_k, \gamma_k$ chosen to fit measured data.
Larger $K \rightsquigarrow$ higher accuracy.

- Results in rational eigenvalue problem

$$Gu - \omega^2 M_1 u - \omega^2 \left(\alpha + \sum_{k=1}^{K} \frac{\xi_k}{\eta_k - \omega^2 - \mathbf{i}\gamma_k\omega}\right) M_2 u = 0. \quad \text{(REVP)}$$

- Task: Compute small eigenvalues of (REVP) close to real axis.

Rational Eigenvalue Problems Solved by Linearization

Linearization via polynomial eigenvalue problems

- Naive approach to linearize rational eigenvalue problem: multiply by all denominators and linearize resulting polynomial eigenvalue problem.

Example (Kádár, Szabó, Volk, 2005):

- Lorentz model with $K = 7$ terms
  for 66% porous silicon
- intermediate polynomial EVP of degree 16
- discretization with FEs of order p

p	size of ... problem	
	original	linearized
2	288	4608
4	720	11520
6	1344	21504
8	2160	34560
12	4368	69888
18	9120	145920

$\rightsquigarrow$ increased execution time and memory consumption

Direct linearization

Direct linearization suggested by [Su/Bai'11] in a nutshell:

(i) Rewrite rational matrix $T(\lambda)$ as

$$T(\lambda) = P(\lambda) - \tilde{T}(\lambda) \quad P \text{ polynomial} \quad \tilde{T} \textit{ proper} \text{ rational}$$

(ii) View $\tilde{T}$ as transfer function matrix $\rightsquigarrow$ realization

$$\tilde{T}(\lambda) = C^T(A - \lambda E)^{-1}B$$

$A, E \in \mathbb{R}^{d\times d}$ with $d =$ McMillan degree of $\tilde{T}(\lambda)$.

(iii) Schur complement trick $\rightsquigarrow$

$$T(\lambda) \mathrel{\hat{=}} \begin{bmatrix} P(\lambda) & C^T \\ B & A \end{bmatrix} - \lambda \begin{bmatrix} 0 & 0 \\ 0 & E \end{bmatrix}$$

(iv) Linearize $P(\lambda)$ to obtain linear eigenvalue problem.

Comparison of the two linearizations

problem size		polynomial linearization		direct linearization	
p	#dofs	size	comp. time (s)	size	comp. time (s)
2	288	1728	15.4	720	6.4
4	720	4320	46.1	1800	16.7
6	1344	8064	116	3360	46.7
8	2160	12960	258	5400	130
12	4368	26208	899	10920	430
18	9120	54720	3471	22800	1424

- Synthetic 2-term Lorentz model.
- Comp. time for 10 smallest eigenvalues of 30 eigenvalue problems (corresponding to 30 different wave vectors), using ARPACK applied to the linearization (shift-and-invert Arnoldi with zero shift).
- Difference becomes more pronounced for larger K and more materials.

Comparison of the two linearizations

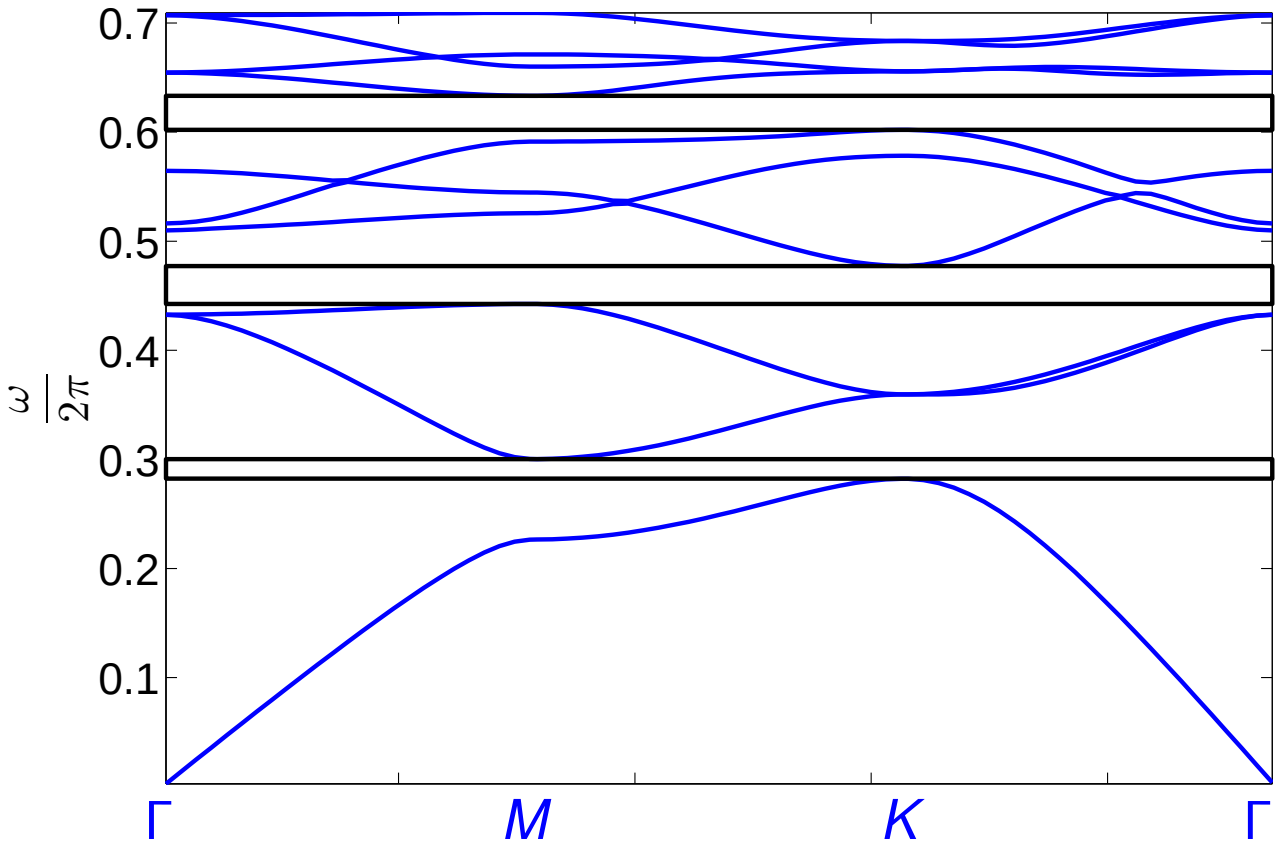
problem size		polynomial linearization		direct linearization	
p	#dofs	size	comp. time (s)	size	comp. time (s)
2	288	4608	—	1584	14.9
4	720	11520	—	3960	35.2
6	1344	21504	—	7392	89.2
8	2160	34560	—	11880	222
12	4368	69888	—	24024	817
18	9120	145920	—	50160	2081

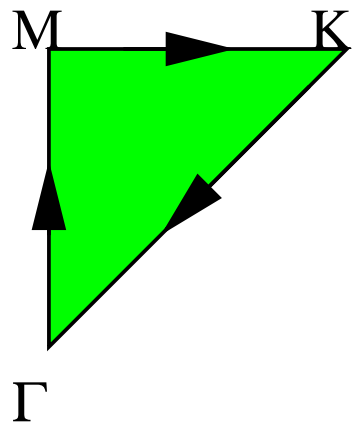
- 7-term Lorentz model for porous silicon
- Formulation of polynomial eigenvalue problem becomes too cumbersome and numerically problematic.

Invariant Pairs for Nonlinear Eigenvalue Problems

Continuation of several eigenvalues

- Idea: Avoid linearization and reuse+refine eigenvalues / eigenvectors obtained from previous wave vector [Spence/Poulton'05].
- Need to represent several eigenvalues / eigenvectors in a robust manner, insensitive to crossings among eigenvalues of interest.





Nonlinear eigenvalue problems

Consider nonlinear eigenvalue problem (NLEVP)

$$\big(f_1(\lambda)A_1 + f_2(\lambda)A_2 + \cdots + f_m(\lambda)A_m\big)x = 0, \quad x \neq 0$$

with $A_1, \ldots, A_m \in \mathbb{C}^{n\times n}$, analytic functions $f_1, \ldots, f_m : \Omega \to \mathbb{C}$.

- In theory, any (finite-dimensional) nonlinear eigenvalue problem $T(\lambda)$ can be written in this form.
- In practice, m should be small: $m \ll n$. (excludes NLEVPs arising from Trefftz-type discretizations, boundary element methods)
- Alternative: contour integral formulation [Beyn'11].

Dealing with several eigenvalues

For simplicity, assume $m = 2$.
Let λ_1, λ_2 be eigenvalues with eigenvectors x_1, x_2:

$$\begin{aligned} \big(f_1(\lambda_1)A_1 + f_2(\lambda_1)A_2\big)x_1 &= 0 \\ \big(f_1(\lambda_2)A_1 + f_2(\lambda_2)A_2\big)x_2 &= 0 \end{aligned}$$

Rearranging terms...

$$\begin{aligned} A_1 x_1 f_1(\lambda_1) + A_2 x_1 f_2(\lambda_1) &= 0 \\ A_1 x_2 f_1(\lambda_2) + A_2 x_2 f_2(\lambda_2) &= 0 \end{aligned}$$

Merging both equations...

$$A_1 \begin{bmatrix} x_1, & x_2 \end{bmatrix} \begin{bmatrix} f_1(\lambda_1) & 0 \\ 0 & f_1(\lambda_2) \end{bmatrix} + A_2 \begin{bmatrix} x_1, & x_2 \end{bmatrix} \begin{bmatrix} f_2(\lambda_1) & 0 \\ 0 & f_2(\lambda_2) \end{bmatrix} = 0$$

Set $X = \begin{bmatrix} x_1, & x_2 \end{bmatrix}$, $S = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$ $\rightsquigarrow$ $A_1 X f_1(S) + A_2 X f_2(S) = 0.$

Invariant pairs

$(X, S) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is called an invariant pair if

$$A_1 X f_1(S) + A_2 X f_2(S) + \cdots + A_m X f_m(S) = 0$$

Remarks:

- For linear eigenvalue problems: $A_1 X - XS = 0 \rightsquigarrow \operatorname{span}(X)$ is invariant subspace belonging to $\Lambda(S)$.
- If S in Jordan canonical form $\rightsquigarrow$ concept of Jordan pairs discussed in classical literature on polynomial/nonlinear eigenvalue problems [Gohberg/Lancaster/Rodman'82, Mennicken/Möller'03].
- Numerical aspects for general S discussed in [Beyn/Thümmler'08] for quadratic EVPs with invertible A_1.
- Extended to general polynomial EVPs in [Betcke/K.'10] and to nonlinear EVPs in [K.'09].

Avoiding degeneracies

Require extra conditions on invariant pairs to avoid degenerate situations, such as $X = 0$.

Is rank$(X) = k$ a reasonable condition?

Example [Dennis/Traub/Weber'76]:

$$\begin{bmatrix} 0 & 12 \\ -2 & 14 \end{bmatrix} + \lambda \begin{bmatrix} -1 & -6 \\ 2 & -9 \end{bmatrix} + \lambda^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The eigenvalues 3 and 4 share the *same* eigenvector $\left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$.

No!

Minimal invariant pairs

Invariant pair $(X, S) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is called minimal (of index ℓ) if

$$V_\ell(X, S) := \begin{bmatrix} X \\ XS \\ \vdots \\ XS^{\ell-1} \end{bmatrix}$$

has full column rank.

For previous example:

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad S = \begin{bmatrix} 3 & 0 \\ 0 & 4 \end{bmatrix}$$

Then

$$V_1(X, S) = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad V_2(X, S) = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 3 & 4 \\ 3 & 4 \end{bmatrix},$$

$V_2(X, S)$ has full column rank $\rightsquigarrow$ (X, S) is minimal.

Minimal invariant pairs

Fundamental properties (polynomial: [Beyn/Thümmler'08], [Betcke/K.'09]; nonlinear [K.'09]):

- For pairwise distinct eigenvalues $\lambda_1, \ldots, \lambda_k$ with eigenvectors $x_1, \ldots, x_k$,

$$(X, S) = \Big(\big[x_1, \ \ldots, \ x_m \big], \operatorname{diag}\big(\lambda_1, \ldots, \lambda_k\big) \Big)$$

  is minimal invariant.
- (X, S) minimal invariant $\rightsquigarrow$ $(XP, P^{-1}SP)$ minimal invariant.
- (X, S) minimal invariant $\rightsquigarrow$ eigenvalues of S are eigenvalues of NLEVP.
- It is always possible to choose $\ell \leq k$.
- Nonminimal pairs (X, S) can be reduced: $\exists$ minimal invariant pair $(\widetilde{X}, \widetilde{S})$ s.t. $\operatorname{span}(\widetilde{X}) = \operatorname{span}(X)$ and $\Lambda(\widetilde{S}) = \Lambda(S)$.

Remark: Structure of $V_\ell(X, S)$ closely related to structures appearing in Krylov subspace methods for solving polynomial eigenvalue problems [Z. Bai and Y. Su. SOAR. SIMAX, 2005].

Newton method for invariant pairs

To develop Newton method for computing/continuing, need operator equations of which (X, S) is a regular value.

$$\mathbb{T}(X, S) = 0 \tag{1}$$

with

$$\begin{aligned} \mathbb{T} : \mathbb{C}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k} &\to \mathbb{C}^{n\times k}, \\ (X, S) &\mapsto XA_1 f_1(S) + \cdots + XA_m f_m(S), \end{aligned}$$

(1) clearly not sufficient to characterize (X, S).

Normalization condition: Choose $W^H = V_\ell(X, S)^\dagger \rightsquigarrow$

$$\mathbb{V}(X, S) = 0 \tag{2}$$

$$\begin{aligned} \mathbb{V} : \mathbb{C}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k} &\to \mathbb{C}^{k\times k}, \\ (X, S) &\mapsto W^H V_\ell(X, S) - I_k. \end{aligned}$$

Linearizing $\mathbb{T}$ and $\mathbb{V}$

Fréchet derivatives of $\mathbb{T}$ and $\mathbb{V}$ at (X, S):

$$\mathbb{DT} : (\triangle X, \triangle S) \quad \mapsto \quad \mathbb{T}(\triangle X, S) + \sum_{j=1}^{m} A_j X \, [\mathbb{D}f_j(S)](\triangle S),$$

$$\mathbb{DV} : (\triangle X, \triangle S) \quad \mapsto \quad W_0^H \triangle X + \sum_{j=1}^{\ell-1} W_j^H \left(\triangle X S^j + X \, \mathbb{D}S^j(\triangle S) \right).$$

Note that the Fréchet derivative of f_j at S can be computed using [Mathias'96, Higham'08]

$$f_j\left(\begin{bmatrix} S & \triangle S \\ 0 & S \end{bmatrix} \right) = \begin{bmatrix} f_j(S) & [\mathbb{D}f_j(S)](\triangle S) \\ 0 & f_j(S) \end{bmatrix}.$$

Is $\mathbb{L} = (\mathbb{DT}, \mathbb{DV})$ *invertible at a minimal invariant pair* (X, S)*?*

Theorem (K.'09)

Let (X, S) *be minimal invariant. The "Jacobian"* $\mathbb{L}$ *of* $(\mathbb{T}, \mathbb{V})$ *at* (X, S) *is invertible if and only if* (X, S) *is simple.*

Remarks:

1. (X, S) is called simple if the algebraic multiplicities of S match those of the NLEVP.
2. Theorem implies local quadratic convergence of Newton iteration applied to $\big(\mathbb{T}(X, S), \mathbb{V}(X, S)\big) = (0, 0)$.

Newton method for computing invariant pairs

Input: Initial pair (X_0, S_0).
Output: Approximate solution (X_{p+1}, S_{p+1}).

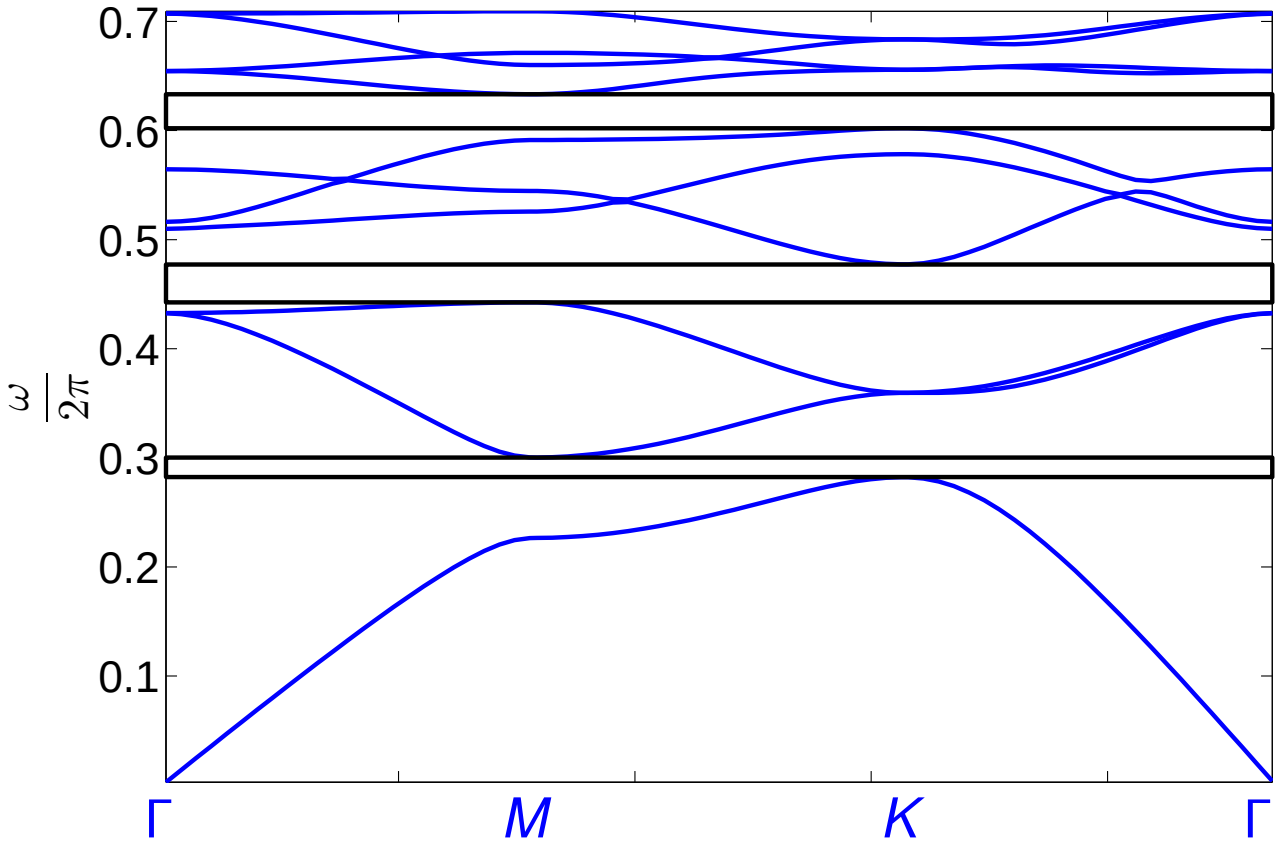
1: $p \leftarrow 0$, $W \leftarrow V_l(X_0, S_0)$
2: **repeat**
3: Res $\leftarrow \mathbb{T}(X_p, S_p)$
4: Solve linear matrix equation $\mathbb{L}_p(\triangle X, \triangle S) = (\text{Res}, 0)$.
5: $\widetilde{X}_{p+1} \leftarrow X_p - \triangle X, \quad \widetilde{S}_{p+1} \leftarrow S_p - \triangle S$
6: Compute compact QR decomposition $V_l(X_p, S_p) = WR$.
7: $X_{p+1} \leftarrow \widetilde{X}_p R^{-1}, \quad S_{p+1} \leftarrow R\widetilde{S}_{p+1}R^{-1}$
8: **until** convergence

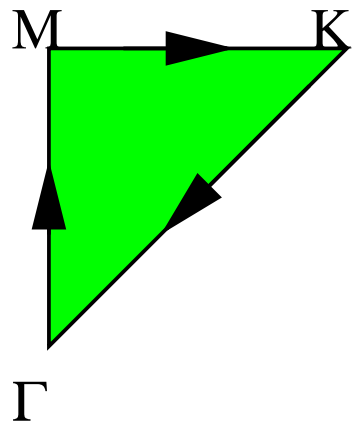
Remarks:

- If no good initial guess available, use smarter algorithm to create one.
- Add simple line search to enhance global convergence properties.
- Step 4 is very expensive, $\mathcal{O}(k^3(n+k)^3)$ flops to solve linear system! After a Schur decomposition of S_p, block lower triangular structure of $\mathbb{L}_p(\triangle X, \triangle S) \rightsquigarrow \mathcal{O}(k(n+k)^3)$ flops.

Electronic band structure calculcation

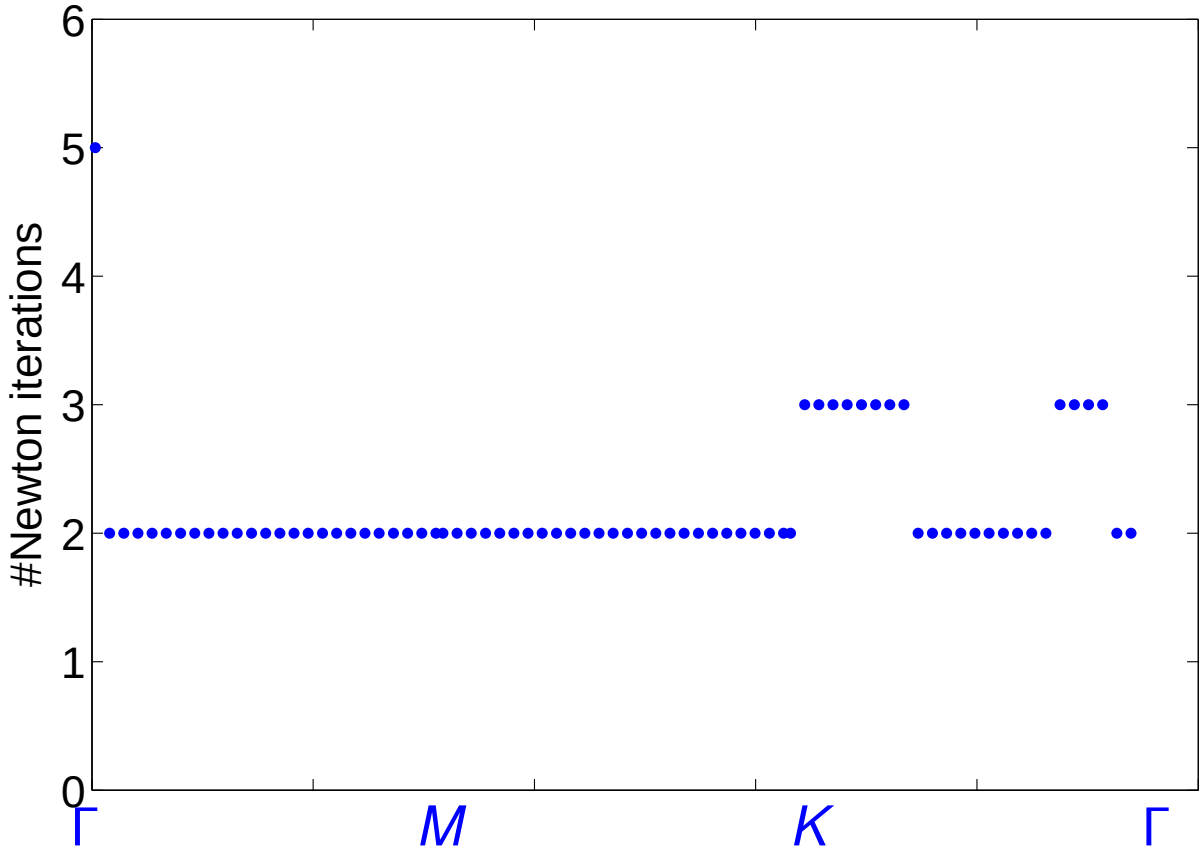
Trace 10 smallest frequencies for 75 equally distributed points on boundary of the Brillouin zone:

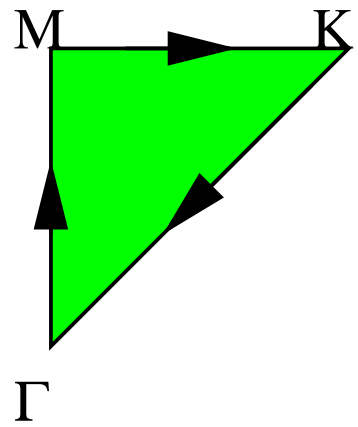




Newton iterations

The computed invariant pair for one wave vector is used to initialize the Newton method for the next wave vector.



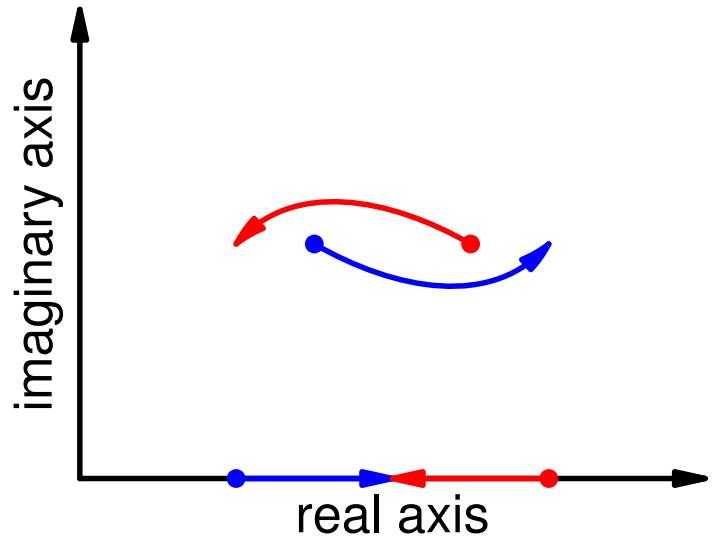


Non-Simple Invariant Pairs

Non-simple invariant pairs

Simple invariant pairs contain all copies of multiple eigenvalues.

- In a parameter-dependent nonlinear eigenvalue problem $T(\lambda, s)$, non-simple invariant pairs occur upon eigenvalue collisions.



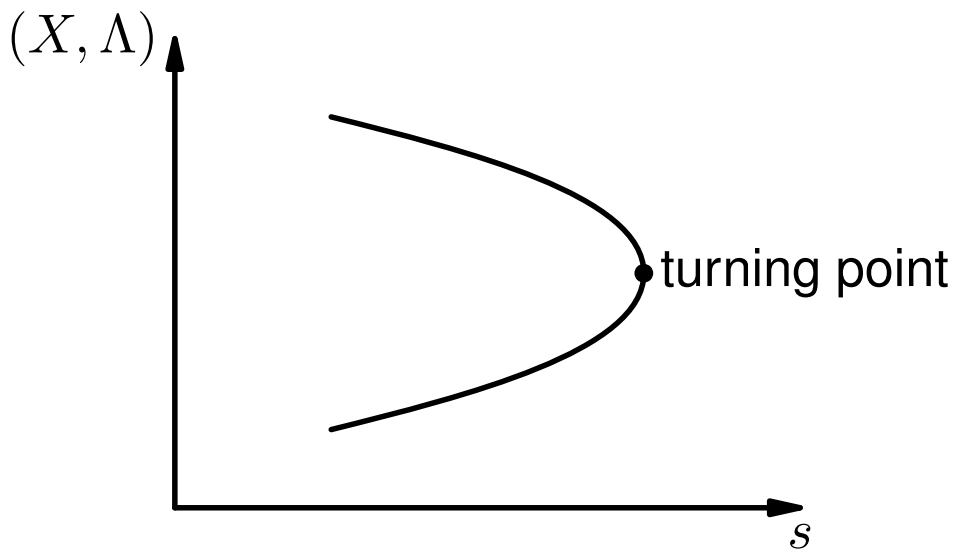
Generic situation for nonsymmetric nonlinear eigenvalue problems:

- Eigenvalue collisions take place on the real axis.
- Typically, the colliding eigenvalues are simple, forming a double, real eigenvalue upon collision.
- After the collision, the eigenvalues move out into the complex plane.

Turning points

Theorem (informal) [Beyn/Effenberger/K.'11]
A generic eigenvalue collision corresponds to a turning point in the solution branch.

Proof based on results for linear case [Beyn/Kleß/Thümmler'01], [Bindel/Demmel/Friedman'08].



The parameterization of the solution branch by s breaks down near a turning point.

Pseudo-arclength continuation

We employ a standard pseudo-arclength continuation method.

- predictor-corrector method
- first-order predictor
- Newton-based corrector
- step length control

Re-parameterization of solution branch

$$(X, \Lambda, s) = (X(t), \Lambda(t), s(t)),$$

where t approximates the arclength of the branch.

Reliable detection of turning points.

Augmenting a non-simple invariant pair

Theorem [Beyn/Effenberger/K.'11]
Let (X_0, Λ_0) be a minimal invariant pair corresponding to a turning point at parameter value s_0. Then,

- the null space of $\mathrm{D}_{(X,\Lambda)}\mathbf{F}(X_0, \Lambda_0, s_0)$ is one-dimensional,
- every basis $(\triangle X_0, \triangle \Lambda_0)$ of the null space has the form

$$\triangle X_0 = x v^\top, \qquad \triangle \Lambda_0 = u v^\top, \qquad v^\top v = 1,$$

- the extended matrices

$$\hat{X}_0 = \begin{bmatrix} X_0 & x \end{bmatrix}, \qquad \hat{\Lambda}_0 = \begin{bmatrix} \Lambda_0 & u \\ 0 & v^\top \Lambda_0 v \end{bmatrix}$$

constitute a simple invariant pair at parameter value s_0.

$$\triangle \Lambda_0 \overset{\text{SVD}}{=} U \Sigma V^\top \qquad \Longrightarrow \qquad u := u_1 \sigma_1, \; v := v_1$$

Academic example

Delay differential equation (Jarlebring, 2008; Wu, 1996)

$$\dot{v}(t) = A_0 v(t) + A_1 v(t-\tau) \qquad \text{(DDE)}$$

with $x_i = \frac{i}{n+1}\pi$ and

$$A_0 = (\tfrac{n+1}{\pi})^2 \begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix} + 20 I_n, \quad A_1 = \operatorname*{diag}_{i=1,\ldots,n} [x_i(1 - \mathrm{e}^{x_i - \pi}) - 4.1]$$

Delay eigenvalue problem

Stability analysis of (DDE) requires a few eigenvalues of

$$(-\lambda I + A_0 + \mathrm{e}^{-\tau\lambda} A_1)x = 0 \qquad \text{(DEVP)}$$

with largest real part.

Solution via continuation

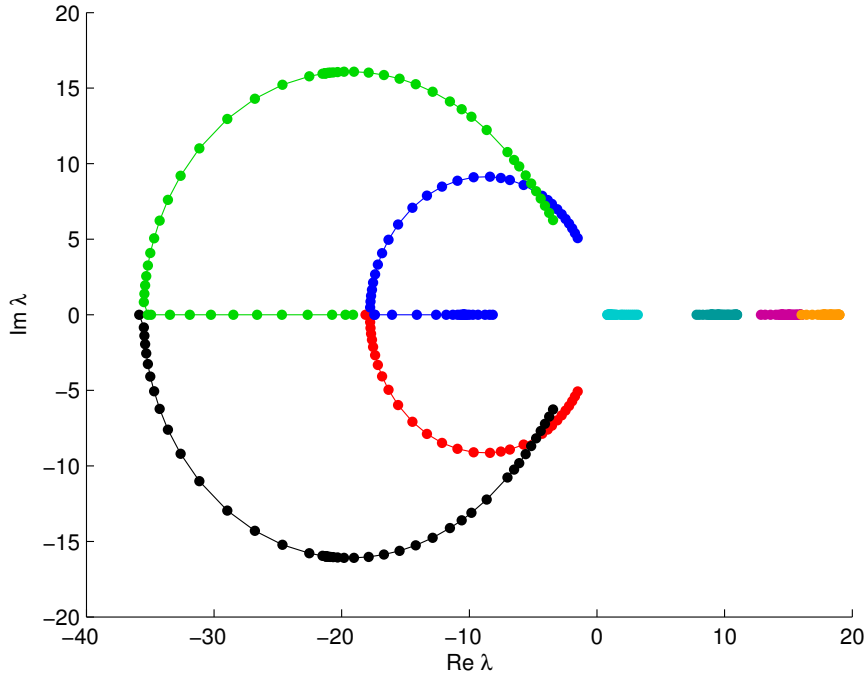
For $\tau = 0$ (no time delay):

- (DEVP) is a symmetric, linear eigenvalue problem.
- easy to solve
- only real eigenvalues

For $\tau > 0$:

- Eigenvalues can be obtained by continuation.
- τ plays role of parameter s
- Some eigenvalues collide and form complex conjugate pairs.

Results


Im λ
Re λ
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−30
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−10
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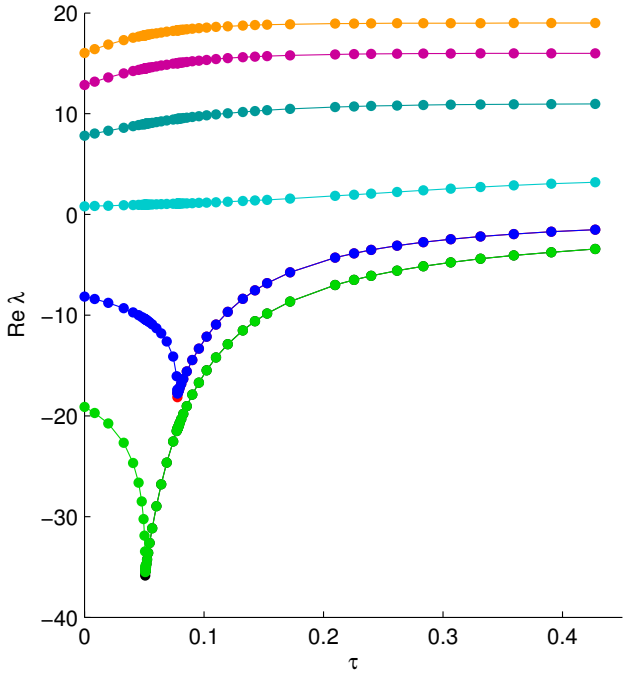
Re λ
τ
20
10
0
−10
−20
−30
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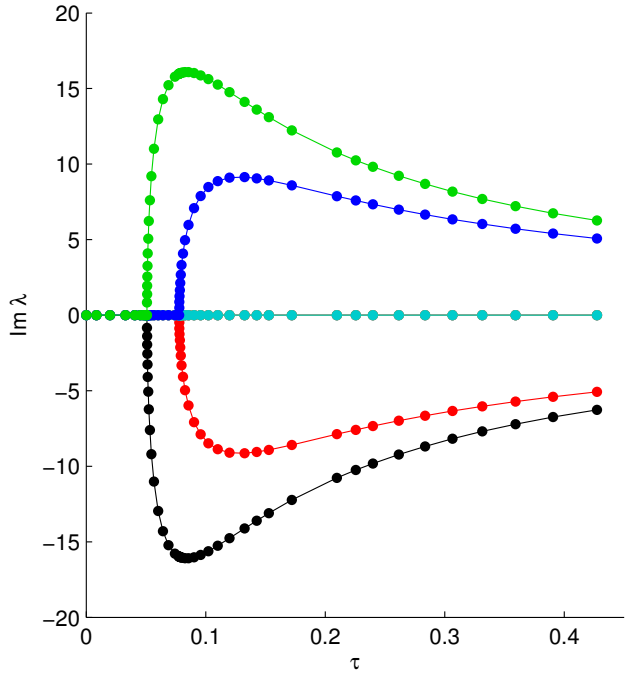
0
0.1
0.2
0.3
0.4


Im λ
τ
20
15
10
5
0
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−15
−20
0
0.1
0.2
0.3
0.4

Conclusion

Summary:

- frequency-dependent material parameters lead to nonlinear eigenvalue problems
- solution of rational eigenvalue problems by linearization
- invariant pairs offer robust representation of several eigenvalues and eigenvectors
- continuation method based on invariant pairs

Future Work:

- large-scale implementation
- structured problems $\rightsquigarrow$ different generic situations
- use of unit cell eigenfunctions in generalized FEM for wave propagation in photonic crystals