From eigenvector nonlinearities to eigenvalue nonlinearities

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Joint work with Elias Jarlebring (KTH)

Outline for this talk

1. Introduction
2. A motivating application
3. Problem statement & method
4. Numerical example
5. Conclusion and outlook

Introduction

We are concerned with **two types of nonlinear eigenvalue problems**, that have both received significant attention in the NLA community.

Problem 1: NEPv (our main problem today)

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$ such that

$$A(v)v = \lambda v, \quad \|v\| = 1,$$

where $A(v) \in \mathbb{R}^{n \times n}$ is symmetric and maps vectors to matrices.

Problem 2: NEP

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$ such that

$$M(\lambda)v = 0,$$

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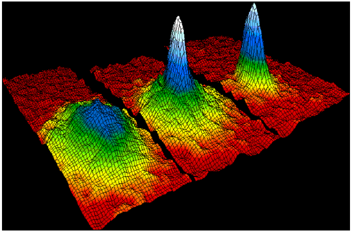
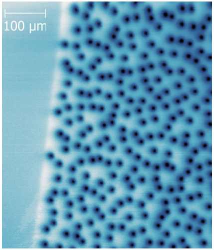
A motivating application: the Gross-Pitaevskii eq.





Left: velocity distribution in condensate. Source: Nobel prize report '01.

Right: quantized vortices in superconductor. Source: Wells et. al. '15.

- Cooling a gas of bosons to ultra-low temperatures results in an exotic state of matter: a **Bose-Einstein condensate**
- Theoretically predicted in 1925 by Bose and Einstein
- Verified experimentally in 1995 → **Nobel prize to Cornell, Ketterle, and Wieman!**
- Modeled by the **Gross-Pitaevskii** equation (GPE)
- Discretization yields **NEPv** with cubic terms

Gross-Pitaevskii eq.

Stationary GPE, continuous setting

Find $u(x)$, $x \in \mathbb{R}^d$, $d = 2, 3$, and $\lambda \in \mathbb{R}$ such that

$$\underbrace{-\Delta u(x)}_{\text{Kinetic energy}} + \underbrace{V_{tr}(x)u(x)}_{\text{Potential energy}} + \underbrace{\kappa|u(x)|^2 u(x)}_{\text{Particle interactions}} = \lambda u(x), \quad \|u\| = 1.$$

Stationary GPE, discrete setting

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$ such that

$$\left(-L_n + D + \kappa\left[(e_1^T v)^2 e_1 e_1^T + \cdots + (e_n^T v)^2 e_n e_n^T\right]\right) v = \lambda v, \quad \|v\| = 1.$$

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Finite differences

See, e.g., [Henning, Målqvist, SIAM J. Numer. Anal. '17], and refs. for more general discretization techniques

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- Symmetric **NEPv**
- **Ground state** typically the smallest eigenvalue, minimizer of the energy in the system
- Often: interested in a few of the smallest eigenvalues
- Challenge: methods for GPE can find the ground state, but no natural way to find several modes

Detour: methods for NEPs

Recall our second problem for today:

Problem 2: NEP

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$ such that $M(\lambda)v = 0$ where $M(\lambda) \in \mathbb{R}^{n \times n}$ is symmetric and maps scalars to matrices.

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- Mature field see e.g. summary [Mehrmann, Voss, GAMM Mitt. '04] or [Güttel, Tisseur, Acta Numerica '17]

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- A wide variety of efficient methods
  - Newton methods: Quasi-Newton, Block-Newton, Broyden's method,...
  - Krylov methods: Rational Krylov, Nonlinear Arnoldi, Infinite Arnoldi,...
  - Jacobi-Davidson methods
  - Contour integral methods: Beyn's method,...
  - Linearization, specialized structures,...

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  - Linearization, specialized structures,...
- Many methods can find several eigenvalues in a natural way

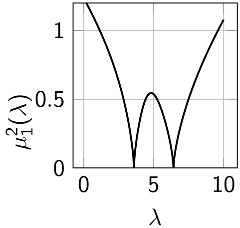
Our approach (simplified case)

GPE-type **NEPv** → Via small poly. sys. → Algebraic **NEP**

$$\left(A_0 + (a_1^T v)^2 a_1 a_1^T\right) v = \lambda v$$

→

$$\left(A_0 + \mu_1^2(\lambda) a_1 a_1^T\right) v = \lambda v$$



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$$\left(\begin{bmatrix}4 & 1\\1 & 6\end{bmatrix} - \lambda I + \left(\begin{bmatrix}3 & 2\end{bmatrix} v\right)^2 \begin{bmatrix}3\\2\end{bmatrix} \begin{bmatrix}3 & 2\end{bmatrix}\right) v = 0$$

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Then $\mu_1^2(\lambda)$ is given explicitly by the function

$$\mu_1^2(\lambda) = \left(\frac{(\lambda^2 - 10\lambda + 23)^2}{13\lambda^2 - 116\lambda + 281}\right)^{2/3},$$

and the **NEP** $\left(A_0 - \lambda I + \mu_1^2(\lambda) a_1 a_1^T\right) v = 0$ can be solved with any **NEP**-solver.

Sketch of transformation

GPE-type **NEPv** (single term)

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$ such that

$$\left(A_0 - \lambda I + (a_1^T v)^2 a_1 a_1^T\right) v = 0, \quad \|v\|^2 = 1,$$

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- Define $\mu_1 = a_1^T v$.
- Distributing v in the eq. above, and using μ_1, gives us

$$(A_0 - \lambda I)v + \mu_1^3 a_1 = 0$$

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- Use the normalization $1 = \|v\|^2 = |\mu_1^3| \, \|(\lambda I - A_0)^{-1} a_1\|^2$
- Finally (use 2-norm and symmetry of A_0):

$$\mu_1^2 = \mu_1^2(\lambda) = \left[\frac{1}{a_1^T (\lambda I - A_0)^{-2} a_1}\right]^{2/3}$$

The general case

GPE-type NEPv

Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$, $m \leq n$, such that

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- The functions $\mu_1(\lambda), \ldots, \mu_m(\lambda)$ are defined implicitly via a **small polynomial system** of m equations in $m+1$ variables.
- It is derived in a fashion similar to the above example. $\rightarrow$ They exist generically under the assumptions of the implicit function theorem.

Defining $\mu_1(\lambda), \ldots, \mu_m(\lambda)$

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$$v = \mu_1^3 (\lambda I - A_0)^{-1} a_1 + \cdots + \mu_m^3 (\lambda I - A_0)^{-1} a_m$$

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- The normalizaition condition gives one eq. We have additionally:

$$(\mu_\ell =)\ a_\ell^T v = \mu_1^3 a_\ell^T (\lambda I - A_0)^{-1} a_1 + \cdots + \mu_m^3 a_\ell^T (\lambda I - A_0)^{-1} a_m,$$

which gives m additional equations, $\ell = 1, \ldots, m$.

Defining $\mu_1(\lambda), \ldots, \mu_m(\lambda)$

Polynomial system

The vector $\mu = [\mu_1, \ldots, \mu_m]^T$ satisfies the relations

$$(\mu^3)^T G(\lambda)\mu^3 - 1 = 0,$$
$$P(H(\lambda)\mu^3 - \mu) = 0,$$

with $G(\lambda) = A_m^T(\lambda I - A_0)^{-2}A_m$, $H(\lambda) = A_m^T(\lambda I - A_0)^{-1}A_m$.

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- $G, H =$ transfer functions
- Note: potentially several solutions for one $\lambda \rightarrow$ Multi-valued functions

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Equivalent **NEP**

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Equivalence

- By construction, **NEPv**-solutions are **NEP**-solutions. The converse also holds:

Theorem (Thm. 2.3, Jarlebring, L., 2025)

The polynomial system generically defines functions $\mu(\lambda) = [\mu_1(\lambda), \ldots, \mu_m(\lambda)]^T$ such that for any (λ_*, v_*), the following two statements are equivalent.

- *The pair (λ_*, v_*) is a solution to the* **NEPv***.*
- *The pair (λ_*, v_*) is a solution to the* **NEP** *with the functions defined by μ and $\|v_*\| = 1$.*

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- The polynomial system must be solved for every evaluation of **NEP** $\rightarrow$ **We need robust solver for polynomial-system**

Solving the polynomial system

$$(\mu^3)^T G(\lambda)\mu^3 - 1 = 0$$
$$P(H(\lambda)\mu^3 - \mu) = 0$$

$w := \mu^3$

$$w^T G(\lambda) w - 1 = 0$$
$$P((H(\lambda)w)^3 - w) = 0$$

"Black box" software
(`HomotopyContinuation.jl`,...)

Reformulation as MEP
(Companion linearization)

$$(A_{10} + w_1 A_{11} + \cdots + w_m A_{1m})x = 0$$
$$\vdots$$
$$(A_{m0} + w_1 A_{m1} + \cdots + w_m A_{mm})x = 0$$

MEP-techniques

Solutions
to poly. syst.
$\to$ **NEP**-eval.

Solving the polynomial system

MEP-formulation of polynomial system

Using a companion linearization, we can write the polynomial equations as

$$\begin{bmatrix} -1 & \boldsymbol{w}^T G^T \\ \boldsymbol{w} & -I_{m\times m} \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{w} \end{bmatrix} = 0$$

$$\begin{bmatrix} -\boldsymbol{w}_k & 0 & h_k^T \boldsymbol{w} \\ h_k^T \boldsymbol{w} & -1 & 0 \\ 0 & h_k^T \boldsymbol{w} & -1 \end{bmatrix} \begin{bmatrix} 1 \\ h_k^T \boldsymbol{w} \\ (h_k^T \boldsymbol{w})^2 \end{bmatrix} = 0$$

with h_k^T being the kth row of $H(\lambda)$, and $k = 1, \ldots, m-1$.

Solving the polynomial system

Transformed system:

$$w^T G(\lambda) w - 1 = 0$$
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- Linear (in $\mathbf{w}_1, \ldots, \mathbf{w}_m$) multi-parameter eigenvalue problem (MEP) $\rightarrow$ **Use standard MEP-methods to obatin all sols.** (operator determinants, generalized eigenvalue problems, cf. [Plestenjak, BIT, '17])

Numerical example (1/4)

We consider a **NEPv** with $m = 5$ nonlinear terms. The problem is derived from an eigenvalue problem in $\mathbb{R}^2$.

GPE-type eigenproblem (continuous setting)

Find $u(x, y)$ and $\lambda \in \mathbb{R}$ such that

$$-\Delta u(x, y) + p(x, y)u(x, y) + \sum_{i=1}^{m} \phi_i^3(u)\psi_m(x, y) = \lambda u(x, y),$$

with $\|u\|_{L^2} = 1$, and where the functionals $\phi_i(u)$ are defined by

$$\phi_i(u) = \int_\Omega \psi_i(x, y)u(x, y)d\Omega.$$

- $p(x, y)$ = potential function, harmonic oscillator + optical lattice
- $\psi_i(x, y)$ = Gaussians localized in different points

Numerical example (2/4)

- Discretize with FDs + trapezoidal rule for integrals
- We get the discrete **NEPv**:

Discrete problem

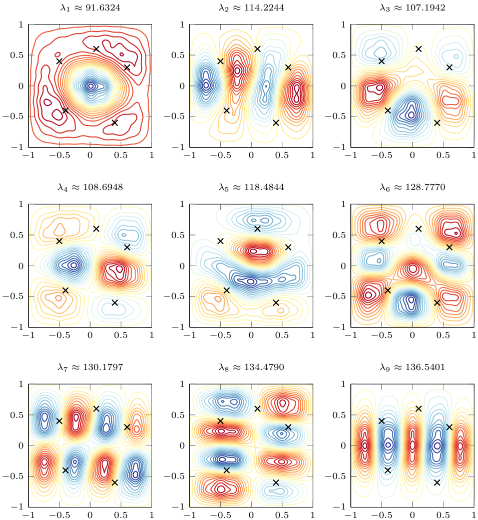
Find eigenpair $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^{N^2}$ such that

$$\left(-L_{N^2} + D + \sum_{i=1}^{m} (a_i^T v)^2 a_i a_i^T \right) v = \lambda v$$

- We solve the **NEPv** by solving the equivalent **NEP**.
- **NEP** solved with Augmented Newton method + deflation of already computed eigs (see, e.g., [Effenberger, '13])

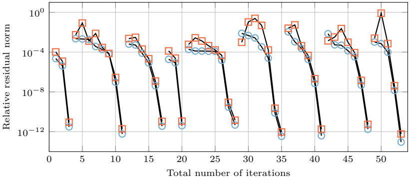
Numerical example (3/4)

Computed eigenmodes:

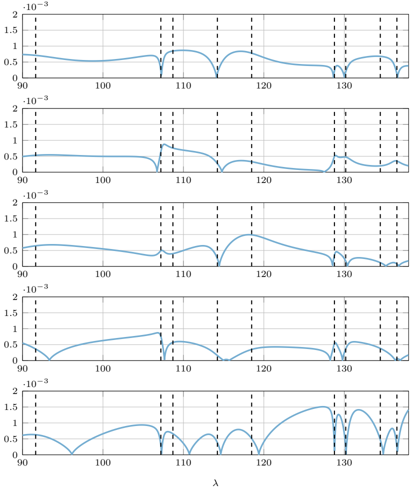


Numerical example (4/4)

Convergence history and μ-functions:



(a) Convergence history



(b) μ-functions

Conclusion

Most important point today: We can solve certain types of **NEPv** by transforming them to an equivalent **NEP**.

Continued work

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- To actually solve the GPE, we need n nonlinear terms. Our approach handles $m \ll n$ comfortably, but $m \approx n$ becomes more difficult.
- Can the GPE be well approximated with only a small number of terms?
- "Easy" generalization: replace squares with more general functions

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Thank you for your attention!

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