Iteration methods for nonlinear PDE eigenvalue problems

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- Linear eigenvalue problem

$$Ax = \lambda\, x$$

- Quadratic eigenvalue problem

$$Ax + \lambda Bx + \lambda^2 Cx = 0$$

- General nonlinear eigenvalue problem

$$F(\lambda, x) = 0$$

- PDE eigenvalue problems

- Linear eigenvalue problem

$$Ax = \lambda\, x$$

- Quadratic eigenvalue problem

$$Ax + \lambda Bx + \lambda^2 Cx = 0$$

- General nonlinear eigenvalue problem

$$F(\lambda, x) = 0$$

- PDE eigenvalue problems
- Two types
  - nonlinearity in the eigenvalue λ
  - nonlinearity in the eigenvector x (eigenvector problem)

1.) Nonlinearity in the **eigenvalue**

→ Example: modeling of photonic crystals

2.) Nonlinearity in the **eigenstate**

→ Example: Bose-Einstein condensates

Nonlinearity in the Eigenvalue

Example: photonic crystals

R. Altmann and M. Froidevaux.
PDE eigenvalue iterations with applications in two-dimensional photonic crystals.
ArXiv Preprint 1905.01066, 2019.

Photonic Crystals

- Special materials, which affect the propagation of electromagnetic waves

$\rightarrow$ used for trapping and guiding light

- Nonlinear eigenvalue problem of Maxwell type
- Crucial parameter: electric permittivity ε

$\rightarrow$ rational function in the frequency = eigenvalue

- Special materials, which affect the propagation of electromagnetic waves

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- Floquet transform, 2D (problem decouples)

$$-\nabla_{\mathbf{k}} \cdot \nabla_{\mathbf{k}} \, u_{\mathbf{k}}(x) = \omega^2 \varepsilon(x,\omega) u_{\mathbf{k}}(x)$$

for a fixed wave vector $\mathbf{k}$, periodic bc

- Here: simple model made up of two different materials

- Lossless case with $\alpha_2 > 0$, $\eta_\ell, \xi_\ell \in \mathbb{R}$,

$$\varepsilon_2(\omega) = \alpha_2 + \sum_{\ell=1}^{L} \frac{\xi_\ell^2}{\eta_\ell^2 - \omega^2}, \qquad \lambda := \omega^2$$

- Eigenvalue problem can be rewritten as

$$\mathcal{A}_{\mathbf{k}} u_{\mathbf{k}} + \Xi\, \mathcal{J}_2 u_{\mathbf{k}} = \lambda\, \mathcal{J} u_{\mathbf{k}} + \mathbf{b}^* \big(\mathbf{A} - \lambda \mathbf{I}\big)^{-1} \mathbf{b}\, \mathcal{J}_2 u_{\mathbf{k}}$$

- Linearization by extension (similar to matrix case)

$$\boldsymbol{x} := (\mathbf{A} - \lambda \mathbf{I})^{-1} \mathbf{b}\, \bar{\mathcal{J}}_2^* u_{\mathbf{k}}$$

→ Equivalent formulation as linear eigenvalue problem

! Based on Gelfand triple with a lack of compactness

- Equivalent linear problem $\mathbb{A} z = \lambda \, \mathbb{I} \, z$ in $\mathcal{V}^*$
- Inverse power method

$$\mathbb{A} z^j = \lambda^{j-1} \, \mathbb{I} \, \tilde{z}^{j-1} \qquad \text{in } \mathcal{V}^*$$

with $\tilde{z}^j = z^j / \|z^j\|_{\mathcal{H}}$ and Rayleigh quotient

$$\lambda^j := \frac{\langle \mathbb{A} z^j, z^j \rangle}{(z^j, z^j)_{\mathcal{H}}}$$

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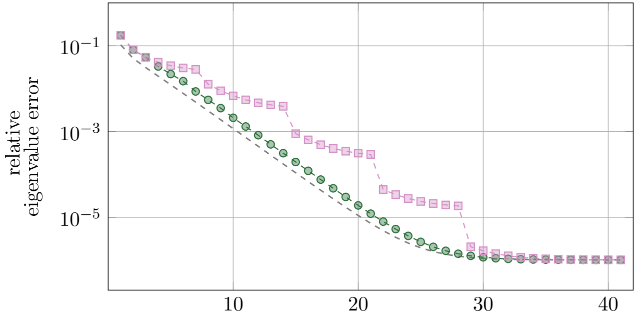
- Convergence result (with compact embedding)
  - subsequence $z^j \to z^\star$ in $\mathcal{V}$, $\lambda^j \to \lambda^\star$
  - $\mathbb{A} z^\star = \lambda^\star \mathbb{I} z^\star$ in $\mathcal{V}^*$
- Without the compactness
  - at least $z^j \rightharpoonup z^\star$ in $\mathcal{V}$, $z^j \to z^\star$ in $\mathcal{H}$

- Inverse power method applied to linearized problem
- Fixed number of iterations per mesh (3: -●-; 7: -■-)
- Iteration on fine mesh (dashed)



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Nonlinearity in the eigenstate

Example: Bose-Einstein condensates

R. Altmann, P. Henning, D. Peterseim.
The J-method for the Gross-Pitaevskii eigenvalue problem.
arXiv:1908.00333, 2019.

- Extreme state of matter in which separate atoms coalesce into a single quantum mechanical entity
- Condensate can be described by a single wave function on a near-macroscopic scale
- 1924: Predicted by Einstein, based on work by Bose

S. Bose. Plancks Gesetz und Lichtquantenhypothese. *Zeitschrift für Physik*, 126(1):178–181, 1924.

A. Einstein. Quantentheorie des einatomigen idealen Gases. *Sitzber. Kgl. Preuss. Akad. Wiss.*, pages 261–267, 1924.

- 1995: Experimental observation

M. Anderson, J. Ensher, M. Matthews, C. Wieman, and E. Cornell. Observation of Bose-Einstein condensation in a dilute atomic vapor. *Science*, 269(5221):198–201, 1995.

- Practical relevance: superfluidity on observable scale

Gross-Pitaevskii Eigenvalue Problem

- Gross-Pitaevskii eigenvalue problem (dimensionless)

$$-\Delta u(x) + V(x)u(x) + \kappa\,|u(x)|^2 u(x) = \lambda\, u(x)$$

  in $D = (0,1)^d$ with hom. Dirichlet bc, $\kappa \geq 0$

- Eigenstate u equals stationary quantum state
- Trapping potentials V:
  - harmonic potential $V(x,y,z) = \gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2$
  - Kronig-Penney potential (discontinuous checkerboard)
    applications: quantum self-trapping, Josephson effect
  - laser speckle (disorder) potentials
    applications: atom optics

- Energy $E(v) := \frac{1}{2}\int_D |\nabla v|^2 + V\,|v|^2 + \frac{\kappa}{2}|v|^4 \,\mathrm{d}x$
- Hilbert space X with inner product $(\,\cdot\,,\cdot\,)_X$

- **Sobolev gradient of E w.r.t. X:**

$$(\nabla_X E(z), v)_X = \langle E'(z), v\rangle \qquad \text{for all } v \in X$$

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- **Projected Sobolev gradient flow:**

$$\dot z(t) = -(P_{z(t),X} \circ \nabla_X E)\, z(t), \quad t \geq 0, \quad z(0) = z_0,$$

where $P_{z(t),X}$ denotes the X-orthogonal projection onto the tangent space $T_{z,X} := \{v \in X \,|\, (v,z)_{L^2(D)} = 0\}$ of the mass constraint

→ Eigenvalue iteration scheme by time discretization

Iteration Methods for PDE-EVP

R. Altmann

Introduction

nonlinear in eigenvalue

nonlinear in eigenstate

- **Example 1:**
  Projected L^2-gradient flow $(X = L^2(D))$

$$\dot{z}(t) = -A_z z + \frac{\langle A_z z, z\rangle}{\|z\|_X^2} z, \qquad A_z z := (-\triangle + V + \kappa\,|z|^2)z$$

- **Example 2:**
  Projected H_0^1-gradient flow $(X = H_0^1(D))$

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- **Example 2:**
  Projected H_0^1-gradient flow $(X = H_0^1(D))$

- Problems with existing flows:
  - no guaranteed energy reduction or
  - convergence properties lost after time discretization

W. Bao and Q. Du.
Computing the ground state solution of Bose-Einstein condensates by a normalized gradient flow.
SIAM J. Sci. Comput., 25(5):1674–1697, 2004.

- **Example 3:**
  Projected a_z-Sobolev gradient flow $(X = H_0^1(D))$
  based on an inner product, which depends on the flow
- Properties:
  - global well-posedness for any normalized $z_0 \in H_0^1(D)$
  - conservation of mass, i.e., $\|z(t)\|_{L^2(D)} \equiv 1$
  - energy reduction
  - convergence and energy reduction remain valid after time discretization for sufficiently small τ (damping parameter)

P. Henning, D. Peterseim.
Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem: global convergence and computational efficiency.
arXiv:1812.00835, 2018.

- Define nonlinear operator A:

$$\langle A(z,v),w\rangle := \int_{\mathcal{D}} \nabla v \cdot \nabla w + V\, v\, w \,\mathrm{d}x + \frac{\kappa}{\|z\|^2} \int_{\mathcal{D}} |z|^2 v\, w\,\mathrm{d}x$$

- Properties of A: $H_0^1(D) \times H_0^1(D) \to H^{-1}(D)$
  - bounded
  - scaling invariant in the first argument
  - linear in the second argument
  - twice Gâteaux differentiable in both arguments

- **GPEVP (A-version):** Find $z^* \in H_0^1(\mathcal{D})$, $\|z^*\| = 1$ and λ^* such that

$$\mathcal{A}(z^*) := A(z^*, z^*) = \lambda^* z^*$$

Iteration Methods for PDE-EVP

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- Consider Gâteaux derivative of $\mathcal{A}$ in $z \in H_0^1(\mathcal{D})$:

$$\langle J(z)v, w\rangle := \langle \mathcal{A}'(z; v), w\rangle$$

- Scaling invariance yields $J(z)z = \mathcal{A}'(z; z) = \mathcal{A}(z)$
- **GPEVP (J-version):** Find $z^* \in H_0^1(\mathcal{D})$, $\|z^*\| = 1$, λ^*

$$J(z^*)z^* = \lambda^* z^*$$

- Example: Gross-Pitaevskii

$$\langle J(z)v, w\rangle = \int_{\mathcal{D}} \nabla v \cdot \nabla w + V\, vw \,\mathrm{d}x + \frac{\kappa}{\|z\|^2} \int_{\mathcal{D}} (zv + 2vz)\, zw \,\mathrm{d}x - \frac{2\kappa\, (z, v)_{L^2(\mathcal{D})}}{\|z\|^4} \int_{\mathcal{D}} |z|^2 zw \,\mathrm{d}x$$

E. Jarlebring, S. Kvaal, W. Michiels,
An inverse iteration method for eigenvalue problems with eigenvector nonlinearities.
SIAM J. Sci. Comput. 36(4):A1978–A2001, 2014.

The J-Method

- **Shifted J-method:** Given $z^0 \in H^1_0(\mathcal{D})$ with $\|z^0\| = 1$ and some shift σ, define

$$z^{n+1} = \frac{(J(z^n) + \sigma)^{-1} z^n}{\|(J(z^n) + \sigma)^{-1} z^n\|}, \quad n \geq 0$$

- **J-method with Rayleigh-shift:** Given z^n, $\|z^n\| = 1$

$$z^{n+1} = \frac{(J(z^n) + \sigma_n)^{-1} z^n}{\|(J(z^n) + \sigma_n)^{-1} z^n\|}, \quad \sigma_n = -\langle \mathcal{A}(z^n), z^n \rangle$$

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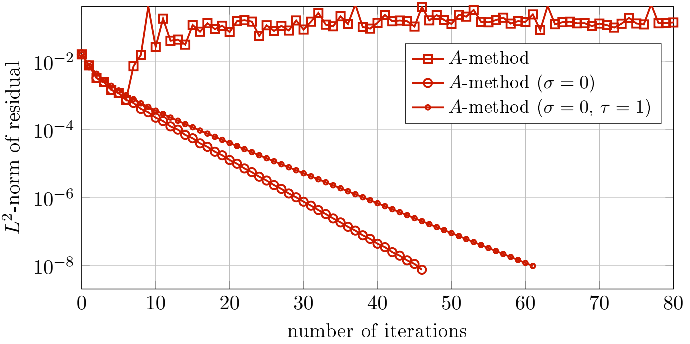
- **Damped J-method:** Given z^n, $\|z^n\| = 1$ and a step size $0 < \tau_n \leq 2$, define

$$\tilde{z}^{n+1} = (1 - \tau_n) z^n + \tau_n \gamma_n \frac{J(z^n)^{-1} z^n}{(J(z^n)^{-1} z^n, z^n)}, \quad z^{n+1} = \frac{\tilde{z}^{n+1}}{\|\tilde{z}^{n+1}\|}$$

- Harmonic potential $V(x) = \frac{1}{2}|x|^2$
- Domain $D = (-L, L)^2$, $L = 8$, $\kappa = 1000$
- FE discretization: Q1 on uniform mesh, $h = 2L \cdot 2^{-8}$



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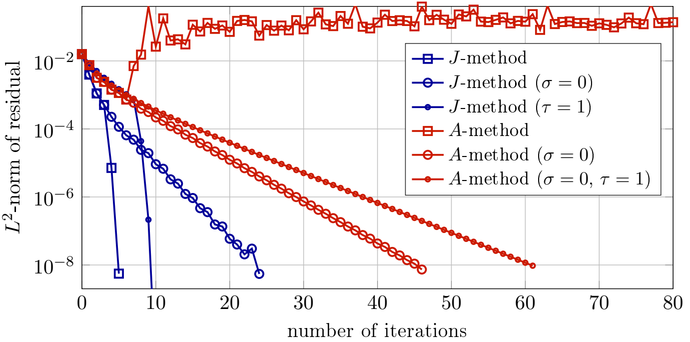

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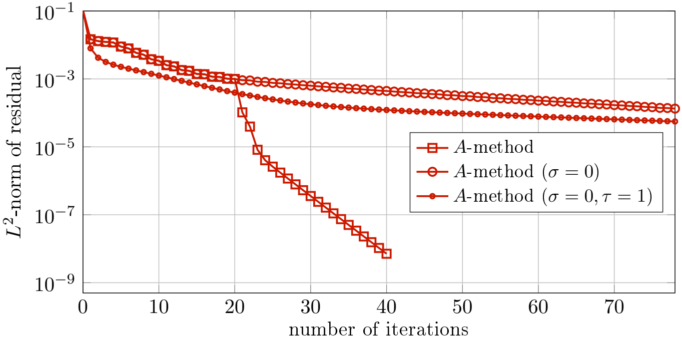
- Random checkerboard potential, $V(x) \in \{0, 2^{12}/(2L)^2\}$
- Domain $D = (-L, L)^2$, $L = 8$, $\kappa = 1$
- FE discretization: Q1 on uniform mesh, $h = 2L \cdot 2^{-8}$



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Numerical Experiment II

Universität Augsburg University

- Random checkerboard potential, $V(x) \in \{0, 2^{12}/(2L)^2\}$
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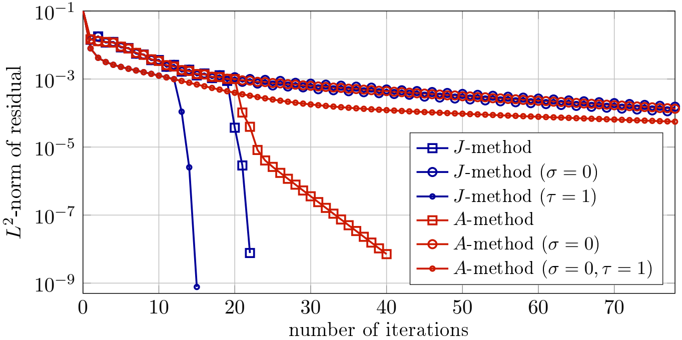

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Conclusion

- Nonlinearity in the eigenvalue

→ exact reformulation by linearization
  - power method in Hilbert space setting
  - allows adaptivity

- Nonlinearity in the eigenvector

→ solvers based on alternative linearization
  - allows spectral shifts
  - acceleration of convergence
  - approximation of excited states, e.g., vortex lattices in fast rotating traps