Numerical approximation of the spectrum of self-adjoint operators and operator preconditioning

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Based on a joint work with
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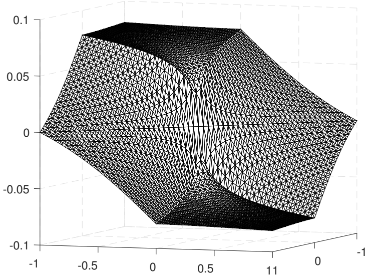
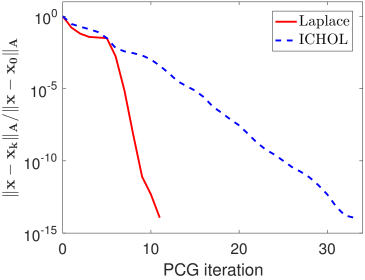
Outline

1. Spectral information and convergence of the conjugate gradient method.
2. Nielsen, Tveito and Hackbusch, *Preconditioning by inverting the Laplacian: An analysis of the eigenvalues* (2009).
3. Gergelits, Mardal, Nielsen and S, *Laplacian preconditioning of elliptic PDEs: Localization of the eigenvalues of the discrete operator* (2019).
4. Gergelits, Nielsen and S, *Generalized spectrum of second order elliptic operators* (2020). Back to the infinite dimensional problem, tensor case.
5. Gergelits, Nielsen and S, *Numerical approximation of the spectrum of self-adjoint operators and operator preconditioning* (2021?).
6. Spectral approximation of operators and/or PDE eigenvalue problems.

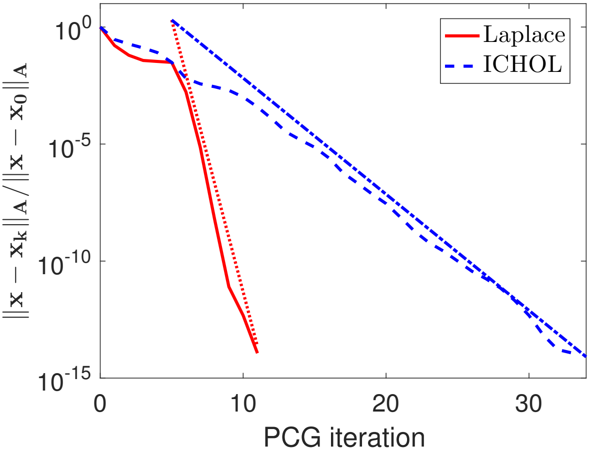




$$-\nabla \cdot (k(x) \nabla u) = 0 ,$$

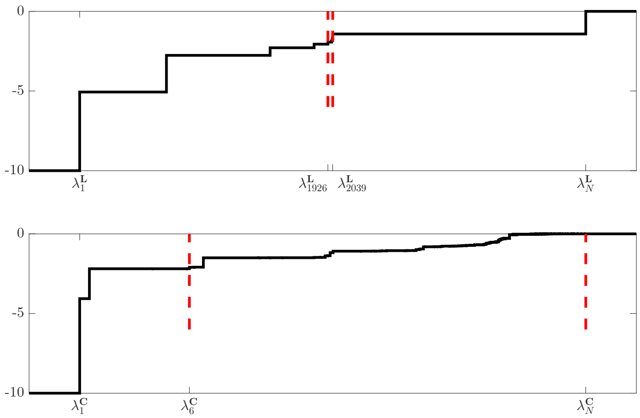
Morin, Nocheto, Siebert, SIREV (2002),
linear FE, standard uniform triangulation, $N = 3969$ DOF.

Conjugate gradients, ICHOL preconditioning (drop-off tolerance 1e-02), $\kappa \approx 16$;
Conjugate gradients, Laplace operator preconditioning, $\kappa \approx 160$.



Laplace
ICHOL
10^{0}
10^{-5}
10^{-10}
10^{-15}
0
10
20
30
PCG iteration
$\|\mathbf{x}-\mathbf{x_k}\|_\mathbf{A}/\|\mathbf{x}-\mathbf{x_0}\|_\mathbf{A}$

1 Distribution functions associated with the discretized problems



(The horizontal scales are different.)

2 Original work that formulated an open problem (2009)

2 Image of the domain under $k(x)$ is included in the spectrum

Consider open and bounded Lipschitz domain $\Omega \in \mathbb{R}^2$ and the operator $\nabla \cdot (k(x)\nabla u)$, where $k(x) : \Omega \to \mathbb{R}$ is a scalar real valued bounded and uniformly positive function. Then for all $x \in \Omega$ at which $k(x)$ is continuous,

$$k(x) \in \mathrm{sp}(\mathcal{L}^{-1}\mathcal{A}),$$

i.e., the image of the domain under a continuous coefficient function $k(x)$ is a subset of the spectrum of the preconditioned operator $\mathcal{L}^{-1}\mathcal{A}$, where

$$\mathcal{A} : H_0^1(\Omega) \mapsto H^{-1}(\Omega), \quad \langle \mathcal{A}u, v\rangle = \int_\Omega k(x)\nabla u \cdot \nabla v, \quad u, v \in H_0^1(\Omega),$$
$$\mathcal{L} : H_0^1(\Omega) \mapsto H^{-1}(\Omega), \quad \langle \mathcal{L}u, v\rangle = \int_\Omega \nabla u \cdot \nabla v, \quad u, v \in H_0^1(\Omega).$$

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Open problem:

Numerical experiments suggest that similar result is valid for the discrete case and that $k(\Omega)$ yields a good approximation of the **whole spectrum** of $\mathcal{L}^{-1}\mathcal{A}$.

3 Discretized problem - a priori localization of all eigenvalues (2019)

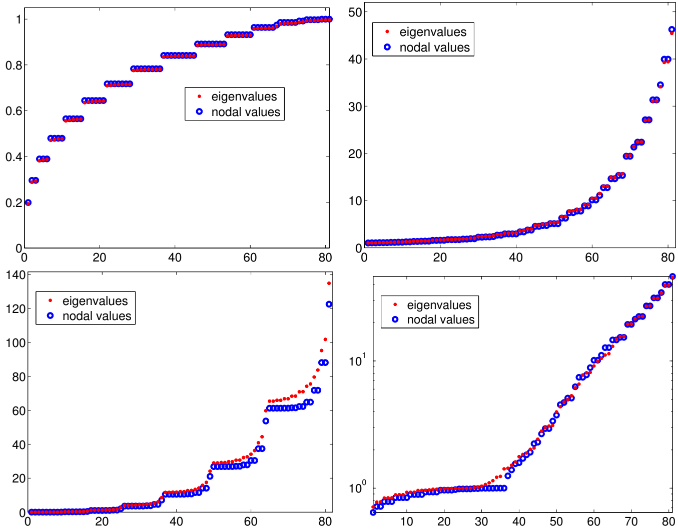
Theorem.

Let $k(x)$ be uniformly positive, bounded and piecewise continuous. Consider discretization via conforming FEM with the basis functions $\phi_j,\ j = 1, \cdots, N$, giving the matrix representations $\mathbf{A}, \mathbf{L}$ of the discrete operators. Let $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$ be the eigenvalues of $\mathbf{L}^{-1}\mathbf{A}$. Then there exists a (possibly non-unique) permutation π such that the eigenvalues of the matrix $\mathbf{L}^{-1}\mathbf{A}$ satisfy

$$\lambda_{\pi(j)} \in k(\mathcal{T}_j), \quad j = 1, \ldots, N,$$

where

$$k(\mathcal{T}_j) \equiv \left[\inf_{x \in \mathcal{T}_j} k(x), \sup_{x \in \mathcal{T}_j} k(x)\right], \quad \mathcal{T}_j = \operatorname{supp}(\phi_j), \quad j = 1, \ldots, N.$$


eigenvalues
nodal values
0
0.2
0.4
0.6
0.8
1
20
40
60
80
10
30
50
70
100
120
140
10^0
10^1

3 Open problems

- Generalizations to tensors, indefinite problems.
- Can the whole spectrum of the infinite dimensional preconditioned operator $\mathcal{L}^{-1}\mathcal{A}$ be determined as $k(\Omega)$?
- 3D: Ivana Pultarová, unpublished note.

4 Determining a priori the operator spectrum (2020)

Consider the operator $\nabla \cdot (K(x)\nabla u)$ with the real valued tensor function $K(x) : \Omega \to \mathbb{R}^{2\times 2}$ being symmetric with its entries being bounded Lebesgue integrable functions, and with the spectral decomposition

$$K(x) = Q(x)\,\Lambda(x)\,Q^T(x)\,, \quad (x) \in \Omega\,,$$

where

$$\Lambda(x) = \begin{bmatrix} \kappa_1(x) & 0 \\ 0 & \kappa_2(x) \end{bmatrix}, \quad QQ^T = Q^T Q = I\,.$$

Theorem.

Let the symmetric tensor $K(x)$ be continuous throughout the closure $\overline{\Omega}$.
Then the spectrum of the operator $\mathcal{L}^{-1}\mathcal{A}$ is given by the interval

$$\mathrm{sp}(\mathcal{L}^{-1}\mathcal{A}) = \mathrm{Conv}(\kappa_1(\overline{\Omega}) \cup \kappa_2(\overline{\Omega}))\,,$$

where

$$\mathrm{Conv}(\kappa_1(\overline{\Omega}) \cup \kappa_2(\overline{\Omega})) = [\,\inf_{x\in\overline{\Omega}} \min_{i=1,2} \kappa_i(x)\}\,,\ \sup_{x\in\overline{\Omega}} \max_{i=1,2} \kappa_i(x)\}\,]\,.$$

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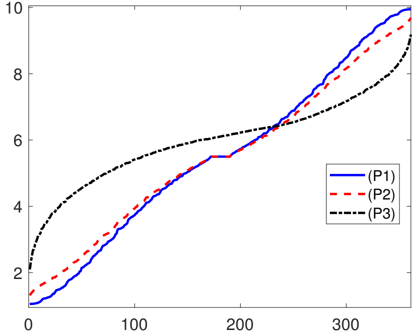
Assuming only that the symmetric tensor $K(x)$ is continuous at least at a single point in Ω and $\sup_{x\in\Omega}\kappa_1(x) < \inf_{x\in\Omega}\kappa_2(x)$, then the following closed interval belongs to the spectrum of $\mathcal{L}^{-1}\mathcal{A}$,

$$[\sup_{x\in\Omega}\kappa_1(x),\; \inf_{x\in\Omega}\kappa_2(x)] \subset \mathrm{sp}(\mathcal{L}^{-1}\mathcal{A}).$$

The analogous statement obviously holds with interchanging κ_1 and κ_2.

4 Eigenvalues of the discretized problems P1 – P3 in the paper



P1: constant $\kappa_1 \neq \kappa_2$
P2: non overlapping $\kappa_1(\overline{\Omega})$ and $\kappa_2(\overline{\Omega})$
P3: overlapping $\kappa_1(\overline{\Omega})$ and $\kappa_2(\overline{\Omega})$

Spectrum of the infinite dimensional preconditioned operator is the complement of the resolvent set. How do the spectra of matrices that represent discretized preconditioned operators approximate the spectral interval of the infinite dimensional preconditioned operator?

Here we do not ask about approximating eigenvalues of the infinite dimensional (PDE) operator by the matrix eigenvalues.

5 Convergence of the matrix eigenvalues towards the whole spectrum

Consider an infinite dimensional Hilbert space V, its dual $V^{\#}$, and bounded linear operators $\mathcal{A}, \mathcal{B} : V \to V^{\#}$ that are self-adjoint with respect to the duality pairing, and $\mathcal{B}$ is, in addition, also coercive. Consider further a sequence of subspaces $\{V_n\}$ of V satisfying the approximation property

$$\lim_{n\to\infty} \inf_{v\in V_n} \|w - v\| = 0 \quad \text{for all } w \in V.$$

Note that this typically yields that Galerkin discretizations of boundary value problems are convergent.

Theorem.

Let the sequences of matrices $\{\mathbf{A}_n\}$ and $\{\mathbf{B}_n\}$ be defined via the standard Galerkin discretization. Then all points in the spectrum of the preconditioned operator

$$\mathcal{B}^{-1}\mathcal{A} : V \to V$$

are approximated to an arbitrary accuracy by the eigenvalues of the preconditioned matrices in the sequence $\{\mathbf{B}_n^{-1}\mathbf{A}_n\}$.

That is, for any point $\lambda \in \mathrm{sp}(\mathcal{B}^{-1}\mathcal{A})$ and any $\epsilon > 0$, there exists n^* such that for all $n \geq n^*$ the preconditioned matrix $\mathbf{B}_n^{-1}\mathbf{A}_n$ has an eigenvalue $\lambda_{j(n)}$ satisfying $|\lambda - \lambda_{j(n)}| < \epsilon$.

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Here we approximate the spectrum of the bounded and continuously invertible operator $\mathcal{B}^{-1}\mathcal{A} : V \to V$ on the infinite dimensional Hilbert space.

6 Spectral theory of operators and PDE eigenvalue problems

6 Compact PDE setting and bounded continuously invertible operators

- PDE eigenvalue problem is based on construction of *compact solution operators.* Babuška - Osborn theory.
- The set of compact operators is closed wrt the norm-wise (uniform) convergence.
- Spectrum of an infinite dimensional compact operator is composed of isolated eigenvalues with a single accumulation point.

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- PDE eigenvalue problem is based on construction of *compact solution operators.* Babuška - Osborn theory.
- The set of compact operators is closed wrt the norm-wise (uniform) convergence.
- Spectrum of an infinite dimensional compact operator is composed of isolated eigenvalues with a single accumulation point.
- Bounded continuously invertible operator on an infinite dimensional Hilbert space is not compact.
- Convergence of matrix eigenvalues to eigenvalues of a compact operator is a different problem than approximation of the whole spectral interval.
  The later, not the former, is crucial in the operator preconditioning.

6 Remarkable history related to Krylov subspace methods

- Euclid (300BC), Hippassus from Metapontum (before 400BC), ... ,
- Bhascara II (around 1150), Brouncker and Wallis (1655-56):
  Three term recurrences (for numbers)
- Euler (1737, 1748), ... , Khrushchev (2008)
  Claude Brezinski (History of Continued Fractions and Padé Approximants (1991)),
- Gauss (1814), Jacobi (1826), Christoffel (1858, 1857), ... ,
  Chebyshev (1855, 1859), Markov (1884), Stieltjes (1884, 1893-94):
  Orthogonal polynomials, quadrature, analytic theory of continued fractions, problem of moments, minimal partial realization, Riemann-Stieltjes integral
  Gautschi (1981, 2004), **Claude Brezinski (1991),** Van Assche (1993), Kjeldsen (1993)
- Hilbert (1906, 1912), ... , Von Neumann (1927, 1932), Wintner (1929):
  resolution of unity, integral representation of operator functions, mathematical foundation of quantum mechanics

- Krylov (1931), Lanczos (1950, 1952, 1952c), Hestenes and Stiefel (1952), Rutishauser (1953), Henrici (1958), Stiefel (1958), Rutishauser (1959), ... , Vorobyev (1954, 1958, 1965), **Claude Brezinski (Methods of Vorobyev and Lanczos (1996)),** Golub and Welsch (1968), ... , Laurie (1991 - 2001), ...

- Gordon (1968), Schlesinger and Schwartz (1966), Steen (1973), Reinhard (1979), ... , Horáček (1983 - ...), Simon (2007 - ...)

- Paige (1971, 1972, 1976, 1980), Reid (1971), Greenbaum (1989), ...

- Magnus (1962a,b), Gragg (1974), Kalman (1979), Gragg, Lindquist (1983), Gallivan, Grimme, Van Dooren (1994), ...

6 Wallis, Arithmetica Infinitorium (1656) (see Khruschev 2008)

"There remains this: we beech the skilled in these things, that we thought worth showing, they will think openly receiving, and whatever it hides, worth imparting more properly by themselves to the wider mathematical community."

Dear Claude,

thank you very much for all what you have done for us!