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

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Based on a joint work with
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Hierarchy of linear problems starting at infinite dimension

Problem with bounded invertible operator $\mathcal{G}$ on the infinite dimensional Hilbert space S

$$\mathcal{G}\, u \;=\; f$$

is approximated on a finite dimensional subspace $S_h \subset S$ by a problem with the finite dimensional operator

$$\mathcal{G}_h\, u_h \;=\; f_h\,,$$

represented, using an appropriate basis of S_h, by the matrix problem

$$\mathbf{A}\,\mathbf{x} \;=\; \mathbf{b}\,.$$

Polynomial (Krylov subspace) methods

(Infinite dimensional) Krylov subspace methods at the step n implicitly construct the finite dimensional approximation $\mathcal{G}_n$ of $\mathcal{G}$ which determines the desired approximate solution $u_n \in u_0 + \mathcal{K}_n(\mathcal{G}, r), \quad r = f - \mathcal{G}u_0$

$$u_n := u_0 + p_{n-1}(\mathcal{G})\, r \;\approx\; u = \mathcal{G}^{-1} f\,.$$

Here $p_{n-1}(\lambda)$ is the associated polynomial of degree at most $n-1$ and $\mathcal{G}_n$ is obtained by restricting and projecting $\mathcal{G}$ onto the nth Krylov subspace

$$\mathcal{K}_n(\mathcal{G}, r) := \operatorname{span}\left\{r, \mathcal{G}r, \ldots, \mathcal{G}^{n-1}r\right\}.$$

A.N. Krylov (1931), Gantmakher (1934), Hestenes and Stiefel (1952), Lanczos (1952-53); Karush (1952), Hayes (1954), Stesin (1954), Vorobyev (1958)

Approximation polynomial for the Krylov subspace method M

From

$$r_n^{\mathrm{M}} \;=\; f \,-\, \mathcal{G}\, u_n^{\mathrm{M}} \;=\; r \,-\mathcal{G}\, p_{n-1}^{\mathrm{M}}(\mathcal{G})\, r =: \; \varphi_n^{\mathrm{M}}(\mathcal{G})\, r$$

we get the approximation polynomial

$$\varphi_n^{\mathrm{M}}(\lambda) = \, 1 \,-\, \lambda\, p_{n-1}^{\mathrm{M}}(\lambda)\,,$$

which is nonlinear both in $\mathcal{G}$ (obvious) and f (through the orthogonality/optimality property defining the particular method M). Clearly

$$\varphi_n^{\mathrm{M}}(0) \;=\; 1\,.$$

Remarkable history related to the conjugate gradient and Lanczos methods

- Euclid (300BC), Hippassus from Metapontum (before 400BC): Greatest common divisor, ...
- Bhascara II (around 1150), Brouncker and Wallis (1655-56): Continued fractions, three term recurrences (for numbers), ...
- Euler (1737, 1748): Continued fraction for functions, ... Khrushchev (2008), 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), Brezinski (1991), Van Assche (1993), Kjeldsen (1993)
- Hilbert (1906, 1912), ... , Von Neumann (1927, 1932), Wintner (1929): Resolution of unity, spectral representation of operator functions, mathematical foundation of quantum mechanics, ...

Matrix computation and control theory context

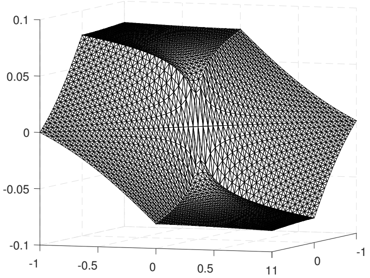
- Krylov (1931), Lanczos (1950, 1952, 1952c), Hestenes and Stiefel (1952), Rutishauser (1953), Henrici (1958), Stiefel (1958), Rutishauser (1959), ... , Vorobyev (1954, 1958, 1965), Brezinski (Methods of Vorobyev and Lanczos (1996)), Golub and Welsch (1968), ... , Laurie (1991 - 2001): Methods, conection to moments, continued fractions, quadrature, ...

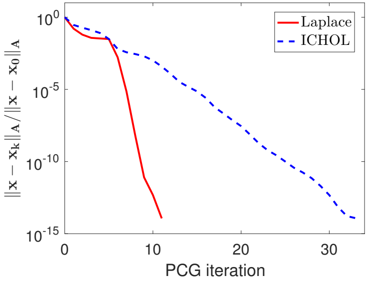
- Gordon (1968), Schlesinger and Schwartz (1966), Steen (1973), Reinhard (1979), ... , Horáček (1983 - ...), Simon (2007 - ...): Mathematical physics, ...

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

- Magnus (1962a,b), Gragg (1974), Kalman (1979), Gragg, Lindquist (1983), Gallivan, Grimme, Van Dooren (1994): Control theory, linear dynamical systems, ...

Motivation: Class of elliptic PDEs, frequently used example, PCG





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

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, $\kappa \approx 160$.

1 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* (SINUM, 2019).
4. Gergelits, Nielsen and S, *Generalized spectrum of second order elliptic operators* (SINUM, 2020). Back to the infinite dimensional problem, tensor case.
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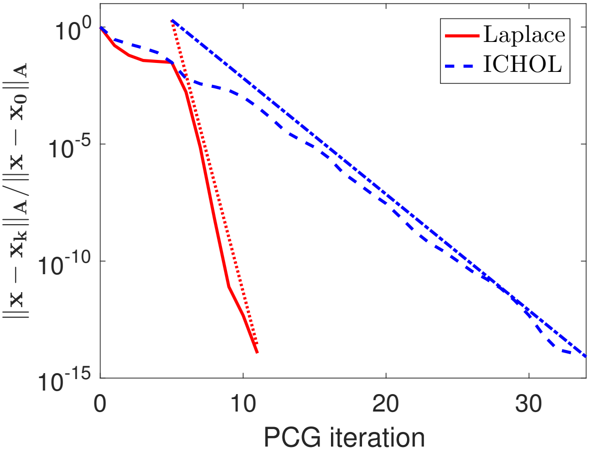
6. Spectral approximation of operators and/or PDE eigenvalue problem.

1 This convergence behaviour does not match the common wisdom!



1 Spectral representation of the operator and the distribution function

Any self-adjoint operator $\mathcal{G}$ defined on V can be expressed in terms of the Riemann-Stieltjes integral as

$$\mathcal{G} = \int \lambda \, dE(\lambda), \quad \text{i.e.} \quad (\mathcal{G}u, v) = \int \lambda \, d(E(\lambda)u, v) \text{ for all } u, v \in V \,,$$

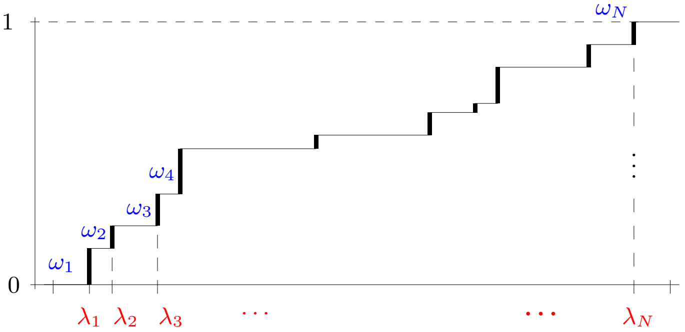
The spectrum of $\mathcal{G}$ is defined as the complement of the resolvent set, i.e.,

$$\mathrm{sp}(\mathcal{G}) = \{\lambda \in \mathbb{R}; \lambda I - \mathcal{G} \text{ does not have a bounded inverse}\} \,.$$

The distribution function $\omega(\lambda)$ is defined by $\mathcal{G}$ and the normalized initial residual $r, \|r\| = 1$ as

$$(\mathcal{G}r, r) = \int \lambda \, d(E(\lambda)r, r) = \int \lambda \, d\omega(\lambda) \,.$$

$\lambda_i, \mathbf{y}_i$ are the eigenpairs of $\mathbf{A}$, $\omega_i = |(\mathbf{y}_i, \mathbf{w}_1)|^2$, $\quad (\mathbf{w}_1 = \mathbf{r}_0/\|\mathbf{r}_0\|)$



1. How is the distribution function determined by the preconditioned system related to the convergence behavior of the conjugate gradient method? What should preconditioning in the case of self-adjoint and coercive operators aim at?

2. What is the relationship between the distribution function of the problem defined on the infinite dimensional Hilbert space and the stepwise distribution functions defined by the associated discretized problems? Or, what is, at least, the relationship between the spectrum of the infinite dimensional (non-compact) operator and the spectra of the associated matrices arising from discretization?

3. Can we *a priori* say anything about the spectra of the matrices arising from discretization?

1 The key concept: CG as the Gauss-Christoffel quadrature.

At any iteration step n, CG represents the matrix formulation of the n-point Gauss quadrature of the Riemann-Stieljes integral determined by $\mathbf{A}$ and $\mathbf{r}_0$,

$$\int_0^\infty \phi(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \phi(\theta_i^{(n)}) \;+\; R_n(\phi)\,.$$

For the function $\phi(\lambda) \equiv \lambda^{-1}$,

$$\frac{\|\mathbf{x}-\mathbf{x}_0\|_{\mathbf{A}}^2}{\|\mathbf{r}_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|\mathbf{x}-\mathbf{x}_n\|_{\mathbf{A}}^2}{\|\mathbf{r}_0\|^2}\,.$$

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Consequence: CG convergence behavior is determined by the approximation of the distribution function $\omega(\lambda)$ determined by the data via the sequence of the Gauss-Christoffel step-wise distribution functions $\omega^{(n)}(\lambda)$, $n = 1, 2, \ldots$

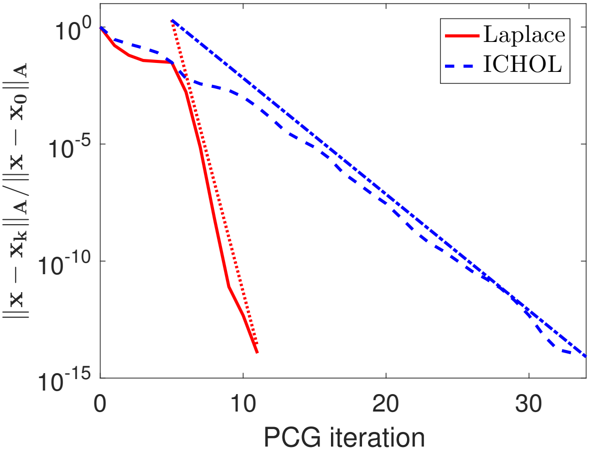
1 CG (Lanczos) in finite precision arithmetic?

Rounding errors seemingly irreparably destroy the underlying mathematical structure that is based on orthogonality, and therefore the link with Gauss-Christoffel quadrature seems to be irreparably lost as well. However,

Lanczos (with small inaccuracy also CG) in finite precision arithmetic can be seen as the exact arithmetic Lanczos (CG) for the problem with the slightly modified distribution function with single eigenvalues replaced by tight clusters.

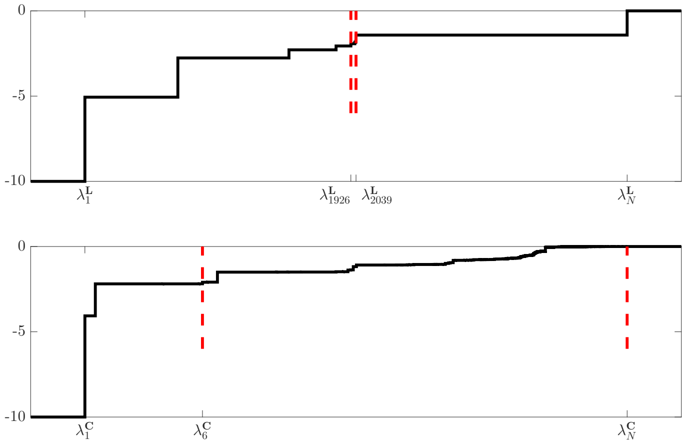
Paige (1971-80), Greenbaum (1989),
Parlett (1990), S (1991), Greenbaum and S (1992), Notay (1993), ... , Druskin, Kniznermann, Zemke, Wülling, Meurant, ...

Reviews and updates in Meurant and S, Acta Numerica (2006); Meurant (2006); Liesen and S (2013).



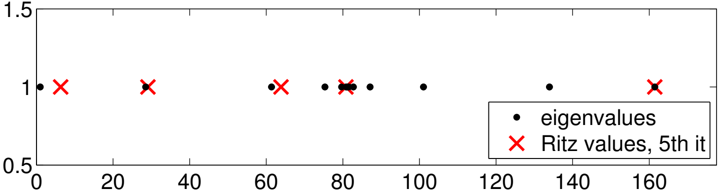
Laplace
ICHOL
10^{0}
10^{-5}
10^{-10}
10^{-15}
0
10
20
30
PCG iteration
$\|\mathbf{x}-\mathbf{x_k}\|_\mathbf{A}/\|\mathbf{x}-\mathbf{x_0}\|_\mathbf{A}$

1 Various parts of the spectra and convergence behavior



The horizontal scales are different.

1 Ritz values at the 5th CG iteration - LAPL

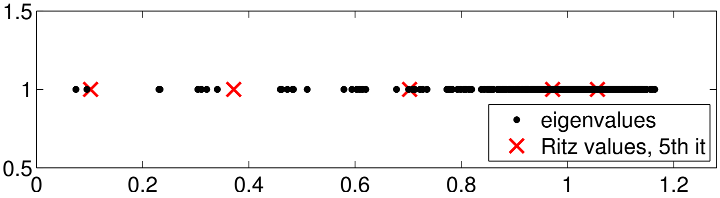


Index	1 – 1922	1923	1924	1925	1926
Eigenvalues	1	28.508	61.384	75.324	$\lambda_{1926}^{\mathbf{L}} = 79.699$
Total weight	9×10^{-6}	$\approx 10^{-3}$	$\approx 10^{-3}$	$\approx 10^{-3}$	$\approx 10^{-3}$

Index	1927 – 1930	1931 – 2039	2040 – 2047	2048 – 3969
Eigenvalues	80.875 – 81.222	$\lambda_{2039}^{\mathbf{L}} = 81.224$	81.226 – 133.94	161.45
Total weight	$\approx 10^{-3}$	1.8×10^{-2}	8×10^{-10}	0.96

Why there are almost two thousand multiple eigenvalues equal to 1 as well as equal to 161.45 ?

1 Ritz values at the 5th CG iteration - ICHOL



Index	1	2	3	4
Eigenvalues	0.074	0.095	0.231	0.233
Total weight	8×10^{-5}	6.4×10^{-3}	8×10^{-7}	10^{-8}

Index	5	6	7 – 3969
Eigenvalues	0.304	$\lambda_6^{\mathbf{C}} = 0.311$	$0.321 - \lambda_{3969}^{\mathbf{C}} = 1.1643$
Total weight	6×10^{-5}	1.5×10^{-3}	0.992

Approximation of the lower end of the spectrum:
van der Sluis, van der Vorst (1986); Liesen, S (2013, Theorem 5.6.9, p. 276).

2 Stimulating work that formulated an open problem (2009)

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).
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6. Spectral approximation of operators and/or PDE eigenvalue problem.

2 Image of the domain under $k(x)$ is a part of the spectrum of $\mathcal{L}^{-1}\mathcal{A}$

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 $k(\Omega)$ yields a good approximation of the **whole spectrum** of $\mathcal{L}^{-1}\mathcal{A}$ and that a similar result is valid for the **spectra of the matrices arising from discretization as well**.

3 Discrete version - a priori localization of all matrix eigenvalues (2019)

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Theorem.

Consider discretization via conforming FEM with the basis functions $\phi_j,\ j = 1, \cdots, N$. Let $\mathbf{A}, \mathbf{L}$ be the matrix representations of the discrete operators. Let $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$ be the eigenvalues of $\mathbf{L}^{-1}\mathbf{A}$. Let $k(x)$ be uniformly positive, bounded and piecewise continuous.

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

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

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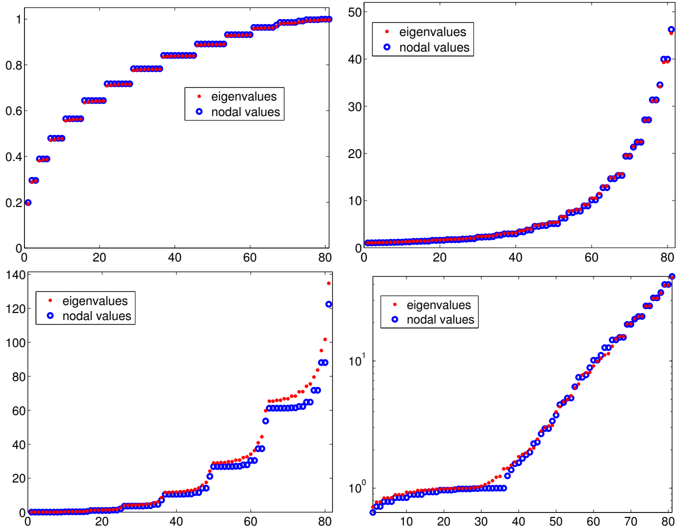
Proof:
Constructive perturbation argument and the Hall's theorem on bipartite graphs.

3 Numerical illustration, 4 problems, nodal values, N = 81



Let $k(\mathcal{T}_j)$ be constant over a patch of the discretization supports.
Then we know the associated eigenvalue exactly including the multiplicity.

Other approach by Ladecký, Pultarová and Zeman (Appl. of Math., 2020).

3 Remark and open problems

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Open questions:

- 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.

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6. Spectral approximation of operators and/or PDE eigenvalue problem.

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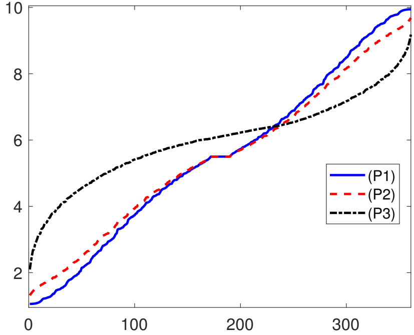
Assuming only that the symmetric tensor $K(x)$ is continuous at least at a single point in Ω and $\sup_{x\in\Omega} \kappa_1(x) < \inf_{x\in\Omega} \kappa_2(x)$, then the following closed interval belongs to the spectrum of $\mathcal{L}^{-1}\mathcal{A}$,

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

The analogous statement obviously holds with interchanging κ_1 and κ_2.



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?
- Relationship with preconditioning? (Instead of approximating the distribution function, here we deal only with approximating the spectrum).

Here we do not ask about numerical approximation of the eigenvalues of the infinite dimensional (PDE) operator, which represents a fundamentally different problem.

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Infinite-dimensional spectrum:

Theorem.

Consider an open and bounded Lipschitz domain $\Omega \subset \mathbb{R}^2$, and the operators $\nabla \cdot (k(x)\nabla u)$, and $\nabla \cdot (g(x)\nabla u)$. Assume that the scalar functions $g(x)$ and $k(x)$ are continuous throughout the closure $\overline{\Omega}$ and that $g(x)$ is, in addition, uniformly positive. Then the spectrum of the operator $\mathcal{B}^{-1}\mathcal{A}$ equals

$$\mathrm{sp}(\mathcal{B}^{-1}\mathcal{A}) = \left[\inf_{x\in\overline{\Omega}} \frac{k(x)}{g(x)}, \sup_{x\in\overline{\Omega}} \frac{k(x)}{g(x)} \right].$$

Eigenvalues of the discretized matrices:

Theorem.

Let $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ be the eigenvalues of $\mathbf{B}_n^{-1}\mathbf{A}_n$. Let $g(x)$ and $k(x)$ be bounded and *piecewise continuous* functions, and $g(x)$ be, in addition, uniformly positive. Then there exists a (possibly non-unique) permutation π such that the eigenvalues of the matrix $\mathbf{B}_n^{-1}\mathbf{A}_n$ satisfy

$$\lambda_{\pi(j)} \in \left[\inf_{x \in \mathcal{T}_j} \frac{k(x)}{g(x)}, \sup_{x \in \mathcal{T}_j} \frac{k(x)}{g(x)} \right], \quad j = 1, \ldots, n,$$

where $\mathcal{T}_j$ represents the support of the jth FEM basis function.

5 Abstract setting (further specific results in the paper)

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 $|\lambda - \lambda_{j(n)}| < \epsilon$.

5 Important point and a question

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.

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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.

Puzzling question:

When the whole spectrum of the infinite dimensional operator is in the limit approximated by the eigenvalues of the associated matrices, and the whole spectrum is a large interval, how can the Laplace preconditioning in the motivating example perform so well? Does it mean that for refined discretizations its performance deteriorates?

The answers are provided by the results above.

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* (Num. Alg., 2022).
6. Spectral approximation of operators and/or PDE eigenvalue problem.

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.

- 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 spectrum of invertible operators. The later, not the former, is relevant to the operator preconditioning.

The presented line of development does not allow to approximate the distribution function $\omega(\lambda)$. Assuming that all eigenspaces contribute to the distribution function equally, we get the so-called *cummulative spectral density,* which is important in physics dealing with the so-called *density of states*; see, e.g., Lin, Saad and Yang, (SIREV, 2016). For the given class of problems we can cheaply approximate this, but the infinite dimensional case is approached only as a limit of the refinements of the discrete cases.

An amazingly beautiful results that do alow to compute (not only) the cumulative spectral density of wide class of infinite dimensional operators are presented in the PhD Thesis by Colbrook (Cambridge U, 2020) and in the several recent related papers; see, in particular, a paper by Colbrook, Horning and Townsend (SIREV, 2021).

"We will go on pondering and meditating, the great mysteries still ahead of us, we will err and stumble on the way, and if we win a little victory, we will be jubilant and thankful, without claiming, however, that we have done something that can eliminate the contribution of all the millenia before us."

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, an whatever it hides, worth imparting more properly by themselves to the wider mathematical community."

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Thank you for your kind attention!