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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GATIPOR, Paris, June 2022

Hierarchy of linear problems starting at infinite dimension

A problem with bounded invertible operator $\mathcal{G}$ on an infinite dimensional Hilbert space V

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

is approximated on a finite dimensional subspace $V_n \subset V$ by a problem with the finite dimensional operator

$$\mathcal{G}_n\, u_n \;=\; f_n\,,$$

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

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

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"There is a continuous operator equation posed in infinite-dimensional spaces that underlines the linear system of equations [...] awareness of this connection is key to devising efficient solution strategies for the linear systems." Hiptmair (2006)

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

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

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

$$\mathcal{K}_j(\mathcal{G}, r) \;:=\; \mathrm{span}\left\{ r, \mathcal{G}r, \ldots, \mathcal{G}^{j-1} r \right\}.$$

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

Approximation polynomial

From

$$r_j = f - \mathcal{G}\, u_j = r - \mathcal{G}\, p_{j-1}(\mathcal{G})\, r =: \varphi_j(\mathcal{G})\, r$$

we get the approximation polynomial

$$\varphi_j(\lambda) = 1 - \lambda\, p_{j-1}(\lambda)\,,$$

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

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

Saad (1981), Greenbaum (1997), Liesen and S (2013)

Preconditioning goes much beyond conditioning

Operator preconditioning

$$\mathcal{G} = \mathcal{B}^{-1}\mathcal{A}$$

where $\mathcal{A}, \mathcal{B} : V \to V^{\#}$ are bounded linear operators on an infinite dimensional Hilbert space V, with its dual $V^{\#}$, and and $\mathcal{B}$ is, in addition, also self-adjoint with respect to the duality pairing and coercive.

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Spectral and norm equivalence may guarantee mesh (parameter) independence, but they do not necessarily provide computational efficiency.

Faber, Manteuffel and Parter (1990), ... , Hiptmair (2006), Málek and S (2015)

Spectrum and its approximation by the finite dimensional eigenvalues

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 standard 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.

Nonuniform convergence of the eigenvalues to all points in the spectrum

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

Descloux, Nassif and Rappaz (1978), Kato (1980), Chatelin (1983), Gergelits, Nielsen and S (2022)

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 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

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

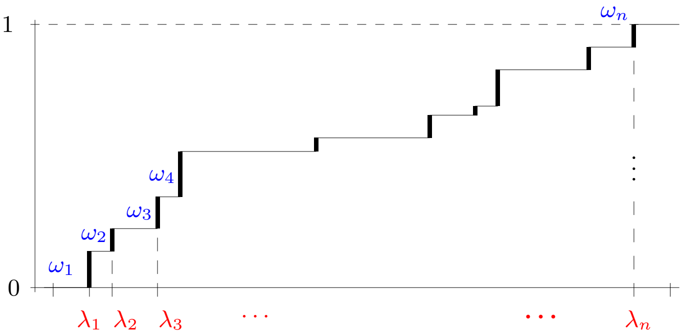
The spectrum of $\mathcal{G}$ is defined as the complement of the resolvent set, i.e.,

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

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

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

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

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

$$\frac{\|\mathbf{x}-\mathbf{x}_0\|_{\mathbf{A}}^2}{\|\mathbf{r}_0\|^2} \;=\; j\text{-point Gauss quadrature} \;+\; \frac{\|\mathbf{x}-\mathbf{x}_j\|_{\mathbf{A}}^2}{\|\mathbf{r}_0\|^2}\,.$$

Consequence: For the discretized problem, CG convergence behavior is determined by the approximations of the distribution function given by $\mathbf{A}, \mathbf{r_0}$ via the sequence of the Gauss-Christoffel step-wise distribution functions $\{\omega^{(j)}(\lambda)\}$.
But this should be linked to the infinite dimensional distribution function $\omega(\lambda)$ determined by $\mathcal{G}, r$.

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).

1 Distribution function (spectrum) and its finite approximations

1. 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?

2. Or, what is, at least, the relationship between the spectrum of the infinite dimensional (non-compact) operator $\mathcal{G}$ and the spectra of the associated (sequence of) matrices arising from (adaptively refined) discretizations?

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

2 Stimulating work that formulated an open problem (2009)

1. Spectral information and convergence of the conjugate gradient method.
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6. Spectral approximation of operators and/or PDE eigenvalue problem.

Theorem.

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

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

2 Open problems formulated in the paper

Numerical experiments suggest that:

1. $k(\Omega)$ yields a good approximation of the whole spectrum of $\mathcal{L}^{-1}\mathcal{A}$;
2. this infinite dimensional spectrum (possibly including its continuous part) is well approximated by the eigenvalues of matrices arising from discretization.

3 Discrete version - a priori localization of all matrix eigenvalues

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

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

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

3 Each cell in the mesh is assigned a different eigenvalue (2019)

Theorem.

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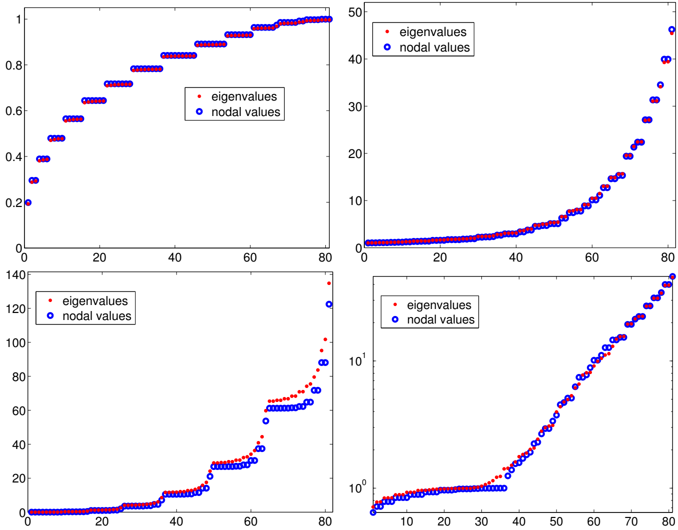
Proof:
Constructive perturbation argument and the Hall's theorem on bipartite graphs.

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



3 Remark and open problems

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:

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

4 Determining a priori the operator spectrum

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.

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

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

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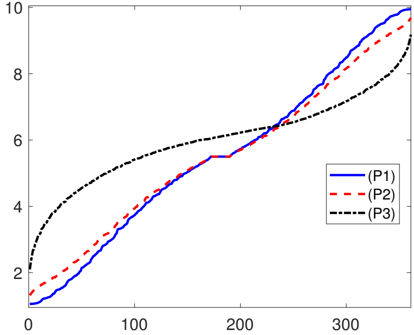
Assuming only that the symmetric tensor $K(x)$ is continuous at least at a single point in Ω and (WLOG) $\sup_{x\in\Omega}\kappa_1(x) < \inf_{x\in\Omega}\kappa_2(x)$, then the following closed interval belongs to the spectrum of $\mathcal{L}^{-1}\mathcal{A}$,

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

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?

- More general 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.

5 Convergence of the matrix eigenvalues towards the whole spectrum

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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 Important point and a question

For the specific cases we get both lower and upper semicontinuity of the spectrum. For the abstract setting we get only lower semicontinuity (see Theorem in part 1).

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, does it mean that for refined discretizations the performance of CG applied to the discretized problems significantly deteriorates with the mesh refinement? Not necessarily! Motivating example in Gergelits, Mardal, Nilesen and S (2019) offers an explanation.

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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.

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.
- 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 finite dimensional distribution functions 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, the 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!