Numerical approximation of the spectrum of self-adjoint operators, operator preconditioning and and unfinished discussion with Radim Blaheta

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Based on a joint work with
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Main topics of our discussions

- Matrix computations using preconditioned Krylov subspace methods
- Relationship with the finite dimensional spectral information
- Effects of rounding errors
- Operator preconditioning in infinite dimensional Hilbert spaces
- Spectral decomposition of infinite dimensional operators and its finite dimensional approximation

Polynomial (Krylov subspace) methods, below $\mathcal{G} = \mathcal{B}^{-1}\mathcal{A},\ f = \mathcal{B}^{-1}b$

Consider a linear equation $\mathcal{G}u = f$ in an infinite dimensional Hilbert space. Infinite dimensional Krylov subspace methods implicitly construct at the step n the finite dimensional approximation 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 the finite dimensional approximation of $\mathcal{G}$ is obtained by the restriction and projection onto the nth Krylov subspace

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

A.N. Krylov (1931), Gantmakher (1934), Hestenes and Stiefel (1952), Lanczos (1952-53); Karush (1952), Hayes (1954), Stesin (1954), Vorobyev (1958), ... , Saad(1996), ...

Approximation polynomial for a 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

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

1 Outline

1. Boundary value problem and operator preconditioning.
2. Spectrum of operators and PDE eigenvalue problem.
3. Spectral information and convergence of the conjugate gradient method.
4. Nielsen, Tveito and Hackbusch, *Preconditioning by inverting the Laplacian: An analysis of the eigenvalues* (2009).
5. Laplacian preconditioning of elliptic PDEs: Localization of the eigenvalues of the discrete operator.
6. Spectrum of preconditioned second order elliptic operators, generalization to indefinite and tensor case.
7. Numerical approximation of the spectrum of self-adjoint operators in operator preconditioning.
8. Concluding remarks.

Consider Hilbert space V with the inner product $(\cdot,\cdot)_V : V \times V \to \mathbb{R}$, $\|\cdot\|_V$, dual space $V^\#$ of bounded linear functionals on V with the duality pairing $\langle\cdot,\cdot\rangle : V^\# \times V \to \mathbb{R}$, and the associated Riesz map

$$\tau : V^\# \to V \quad \text{such that} \quad (\tau f, v)_V := \langle f, v\rangle \quad \text{for all } f \in V^\#,\ v \in V.$$

Consider BVP represented by the equation in the functional space $V^\#$

$$\mathcal{A}u \;=\; b$$

with a linear, bounded, coercive, and self-adjoint operator

$$\mathcal{A} : V \to V^\#, \quad a(u,v) := \langle \mathcal{A}u, v\rangle,$$

$$C_{\mathcal{A}} \;:=\; \sup_{v\in V,\, \|v\|_V=1} \|\mathcal{A}v\|_{V^\#} < \infty,$$

$$c_{\mathcal{A}} \;:=\; \inf_{v\in V,\, \|v\|_V=1} \langle \mathcal{A}v, v\rangle > 0.$$

1 Operator preconditioning defined through the Ritz map

Let a linear, bounded, coercive, and self-adjoint $\mathcal{B}$, $C_{\mathcal{B}}$, $c_{\mathcal{B}}$ be defined analogously,

$$(\cdot,\cdot)_{\mathcal{B}} : V \times V \to \mathbb{R}, \qquad (w,v)_{\mathcal{B}} := \langle \mathcal{B}w, v\rangle \qquad \text{for all } w, v \in V \,,$$

$$\tau_{\mathcal{B}} : V^{\#} \to V, \qquad (\tau_{\mathcal{B}} f, v)_{\mathcal{B}} \;:=\; \langle f, v\rangle \qquad \text{for all } f \in V^{\#},\; v \in V \,.$$

Instead of the original equation in the functional space we can consider the equation in the solution space V

$$\tau_{\mathcal{B}}\, \mathcal{A}\, u \;=\; \tau_{\mathcal{B}}\, b \,,$$

i.e.,

$$\mathcal{B}^{-1}\, \mathcal{A}\, u \;=\; \mathcal{B}^{-1} b.$$

Norm (spectral) equivalence of operators $\mathcal{A}$ and $\mathcal{B}$ is then often used to prove the discretization mesh and problem parameter independence of the resulting (spectral) condition number of the matrix representing the discretized preconditioned operator.

1 Example: Operator preconditioned CG method in Hilbert spaces

For $n = 1, 2, \ldots, n_{\max}$, $\quad (r_0 = f - \mathcal{A}x_0 \in V^{\#}, \quad p_0 = \mathcal{B}^{-1} r_0 \in V)$

$$\alpha_{n-1} = \frac{\langle r_{n-1}, \mathcal{B}^{-1} r_{n-1} \rangle}{\langle \mathcal{A} p_{n-1}, p_{n-1} \rangle}$$

$$x_n = x_{n-1} + \alpha_{n-1} p_{n-1}\,, \qquad \text{stop when the stopping criterion is satisfied}$$

$$r_n = r_{n-1} - \alpha_{n-1} \mathcal{A} p_{n-1}$$

$$\beta_n = \frac{\langle r_n, \mathcal{B}^{-1} r_n \rangle}{\langle r_{n-1}, \mathcal{B}^{-1} r_{n-1} \rangle}$$

$$p_n = \mathcal{B}^{-1} r_n + \beta_n p_{n-1}$$

End

Karush (1952); Hayes (1954); Stesin (1954); Vorobyev (1958, 1965); Daniel (1967, 1967); ... ; Fortuna (1979); Ernst (2000); Axelsson and Karatson (2002); Glowinski (2003); .... ; Zulehner (2011); Günnel, Herzog, and Sachs (2012); ...

1 Discretization of the infinite dimensional CG gives

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$, solve $\mathbf{B}\mathbf{z}_0 = \mathbf{r}_0$, $\mathbf{p}_0 = \mathbf{z}_0$. For $n = 1, \ldots, n_{\max}$

$$
\begin{aligned}
\alpha_{n-1} &= \frac{\mathbf{z}_{n-1}^* \mathbf{r}_{n-1}}{\mathbf{p}_{n-1}^* \mathbf{A}\mathbf{p}_{n-1}} \\
\mathbf{x}_n &= \mathbf{x}_{n-1} + \alpha_{n-1}\mathbf{p}_{n-1}\,, \quad \text{stop when the stopping criterion is satisfied} \\
\mathbf{r}_n &= \mathbf{r}_{n-1} - \alpha_{n-1}\mathbf{A}\mathbf{p}_{n-1} \\
\mathbf{B}\mathbf{z}_n &= \mathbf{r}_n\,, \quad \text{solve for } \mathbf{z}_n \\
\beta_n &= \frac{\mathbf{z}_n^* \mathbf{r}_n}{\mathbf{z}_{n-1}^* \mathbf{r}_{n-1}} \\
\mathbf{p}_n &= \mathbf{z}_n + \beta_n \mathbf{p}_{n-1}
\end{aligned}
$$

Günnel, Herzog, Sachs (2014); Málek, S (2015)

The preconditioned matrix is given by $\mathbf{B}^{-1}\mathbf{A}$, where $\mathbf{A}, \mathbf{B}$ arise from the Galerkin discretization of $\mathcal{A}, \mathcal{B}$ respectively.

1 Operator preconditioning is very important concept, however ...

Hiptmair, CMA (2006):

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.

Operator preconditioning is a very general recipe [...]. It is simple to apply, but may not be particularly efficient, because in case of the [condition number] *bound [...] too large, the operator preconditioning offers no hint how to improve the preconditioner. Hence, operator preconditioner may often achieve [...] the much-vaunted mesh independence of the preconditioner, but it may not perform satisfactorily on a given mesh.*

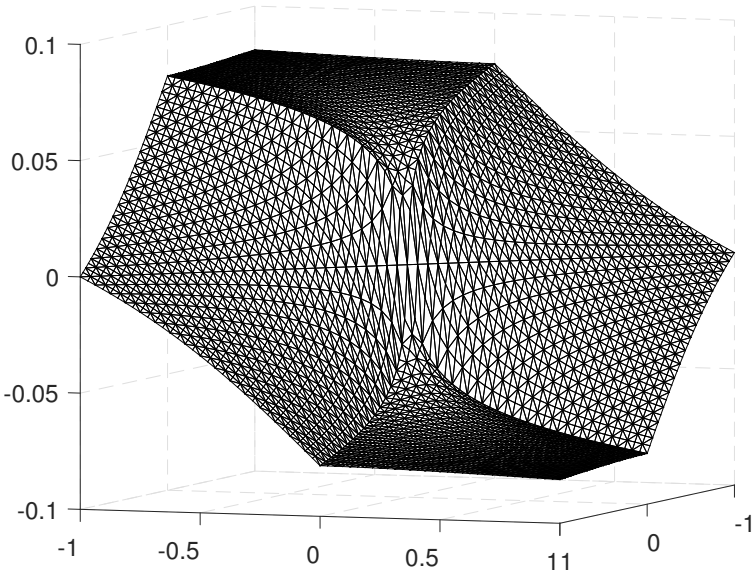
1 Similar warning from an early work

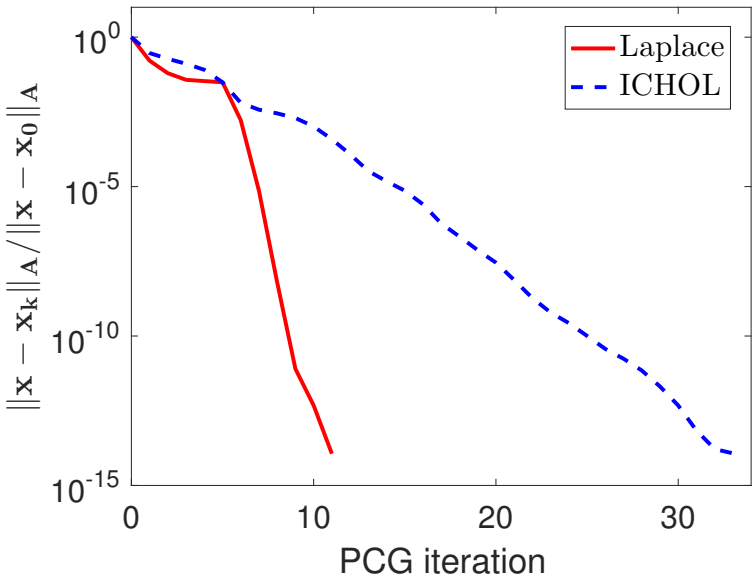
Faber, Manteuffel and Parter, Adv. in Appl. Math. (1990):

For a fixed [discretization parameter] h , *using a preconditioning strategy based on an equivalent operator may not be superior to classical methods [...] Equivalence alone is not sufficient for a good preconditioning strategy. One must also choose an equivalent operator for which the bound is small.*

There is no flaw in the analysis, only a flaw in the conclusions drawn from the analysis [...] asymptotic estimates ignore the constant multiplier. Methods with similar asymptotic work estimates may behave quite differently in practice.

1 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, $\kappa \approx 160$.

2 Spectral representation of operators and eigenvalues

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2 Spectral representation of the operator and the distribution function

Any linear self-adjoint operator $\mathcal{G}$ defined on V can be expressed using the family of spectral projectors $E(\lambda)$ in terms of the Riemann-Stieltjes integral as

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

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

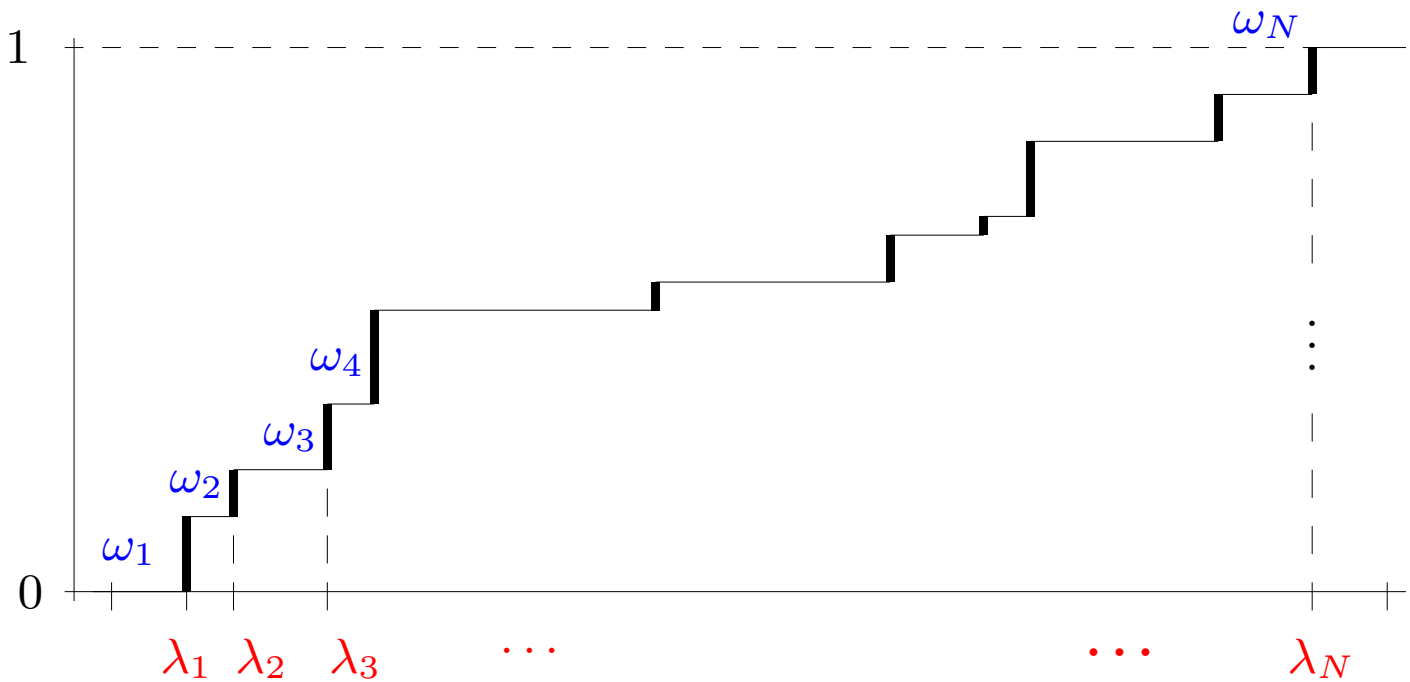
$$\text{sp}(\mathcal{G}) = \{\lambda \in \mathbb{R}; \quad \lambda I - \mathcal{G} \text{ does not have a bounded inverse}\} \,.$$

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

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

cf. von Neumann (1932, 1955) for an instructive exposition of the development of ideas, including the concepts of discrete and continuous spectrum.

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



2 Questions to be addressed

1. How is the distribution function associated with the preconditioned matrix problem related to the convergence behavior of the conjugate gradient method? What are the effects of rounding errors? What should preconditioning in the case of self-adjoint operators aim at?

2. How can we relate the distribution function of the infinite dimensional problem with the stepwise distribution functions defined by the associated discretized problems? Or, what is, at least, the relationship between the spectrum of the infinite dimensional operator (**that is invertible and therefore non-compact**) and the spectra of the associated matrices arising from discretization, which consist of discrete eigenvalues?

3. Can we approximate *a priori* the eigenvalues of matrices arising from discretization?

Hilbert spaces $V \subset H$, $V \neq H$; the proper inclusion is substantial.

Consider a linear, bounded and self-adjoint operator

$$G : V \to V^{\#} , \quad a(u, v) := \langle \mathcal{G}u, v \rangle , \quad \langle \mathcal{G}u, v \rangle , = \langle \mathcal{G}v, u \rangle .$$

The PDE eigenvalue problem then looks for the eigenvalue λ and the eigenvector $w \in V$ associated with $\mathcal{G}$ such that

$$a(w, v) \; = \; \lambda \, (w, v)_H \qquad \text{for all } v \in V .$$

It is resolved through the construction of the **compact operator** $S : H \to V$, such that for any $t \in H$ there is a unique $St \in V$, defined for the given t by

$$a(St, v) \; = \; (t, v)_H \qquad \text{for all } v \in V .$$

- Since S is compact on the infinite dimensional Hilbert space, it is not invertible.
- All its eigenvalues $\{\mu_j\}$ different from zero are isolated.
- The eigenvalues associated with $\mathcal{G}$ are given by $\lambda_j = 1/\mu_j$, $j = 1, 2, ...$

Discretization gives

$$\mathbf{G}\,\mathbf{w} = \lambda\,\mathbf{M}\,\mathbf{w}\,,$$

where $\mathbf{M}$ is the mass (Gram) matrix of the discretization basis wrt the inner product $(w, v)_H$.

Babuška, Osborn (1989, 1991).

3 Spectral information determines CG behavior

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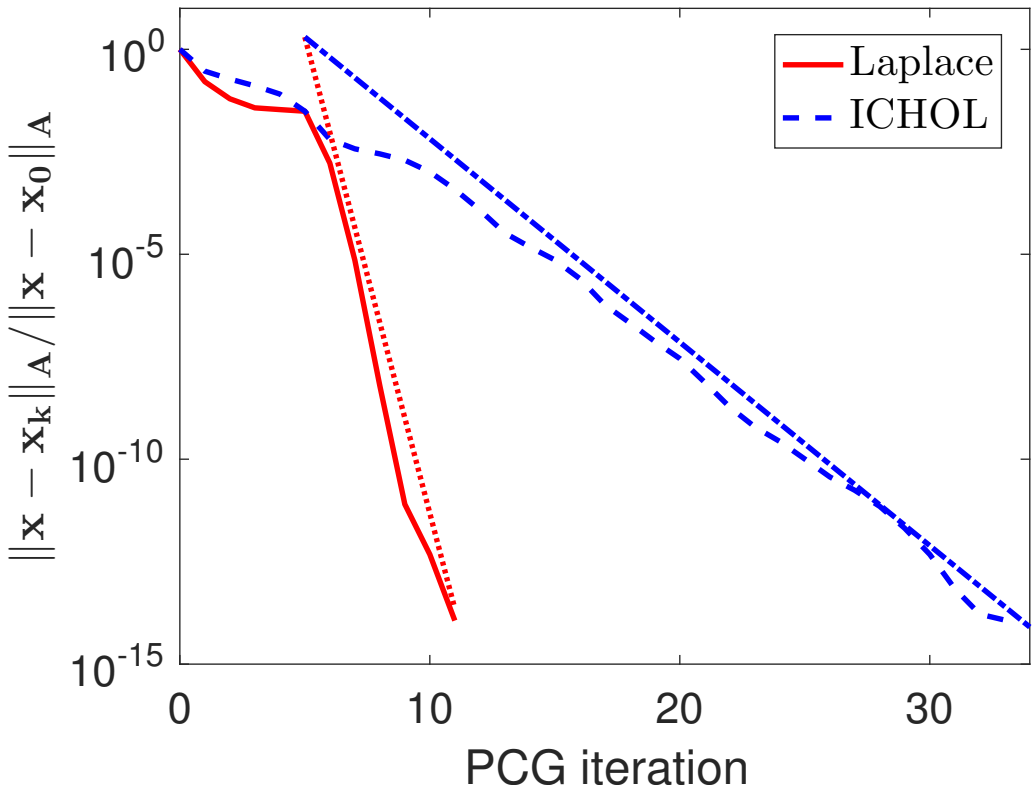
3 The motivating example does not match the common wisdom!



- ICHOL PCG: $\kappa \approx 16$,
- Laplace PCG: $\kappa \approx 160$, rapid linear acceleration after the fifth iteration, slowing down near the maximal attainable accuracy.

3 Back to the originals: Magnus R. Hestenes and Eduard Stiefel (1952)

- Abstract. *An iterative algorithm is given for solving a system $Ax = k$ of N linear equations in N unknowns. The solution is given in N steps. [...] Connections are made with the theory of orthogonal polynomials and continued fractions.*
- Section 3. *At each step the residual $r_i = k - Ax_i$ is computed. Normally this vector can be used as a measure of the "goodness" of the estimate x_i. However, this measure is not a reliable one because [...] it is possible to construct cases in which the squared residual $|r_i|^2$ increases at each step (except for the last) while the length of the error vector decreases monotonically.*
- Section 8. *Propagation of Rounding-Off Errors in the cg-Method.*
- Sections 14. - 17. Orthogonal polynomials, (Riemann)-Stieltjes integral, *mass distribution on the positive axis. [...] During the following investigations we use the Gauss mechanical quadrature as a basic tool ...*

  [Gauss quadrature is equivalent to solving the simplified Stieltjes problem of moments.]
- Section 18. *Continued fractions.*

3 Back to the originals: Cornelius Lanczos (1952)

- *In principle we have obtained a method for the solution of sets of linear equations which is simple and logical in structure. Yet from numerical standpoint we must not overlooked the danger of the possible accumulation of rounding errors.*
- Algorithm I: *purification* of the initial vector of the components in the direction of the eigenvectors corresponding to large eigenvalues using Chebyshev polynomials.
- Algorithm II: minimized iterations equivalent to CG.
- *The principle by which this process* [meant CG] *gives good attenuation is quite different from the previous one* [meant the purification using Chebyshev polynomials]. *The polynomials of this process have the peculiarity that they attenuate due to the nearness of their zeros to those λ-values which are present in A. The advantage of the process is its great economy.*
- *The price we have to pay is that the successive iterations of this process are more complicated than those of algorithm I. Another difficulty arises from the inevitable accumulation of rounding errors.*

3 How does our presence match the visions in these papers?

- Lanczos, Hestenes and Stiefel, as well as Karush, Hayes, and Vorobyev, who considered infinite dimensional Hilbert space setting, made many fundamental points.
- Some were painfully rediscovered (often through computational failures) decades later, other remain unnoticed in literature, including textbooks and monographs, until now.
- The common knowledge on CG is frequently reduced to an algorithmic description without broader context. Convergence rate is viewed through the condition number which results in a linear upper bound based on Chebyshev polynomials. This is sometimes combined with misguided or even plainly wrong arguments on clustering eigenvalues.
- Rounding errors are typically excluded from analysis, while the derived results are claimed to be useful for practical computations.

shifted Chebyshev approximation problem: $\min_{p \in \mathcal{P}_n(0)} \max_{\lambda \in [\lambda_1, \lambda_N]} |p(\lambda)|$

CG approximation problem $\|x - x_j\|_A^2 = \|r_0\|^2 \sum_{\ell=1}^{N} \omega_\ell \frac{(\varphi_j(\lambda_\ell))^2}{\lambda_\ell}$

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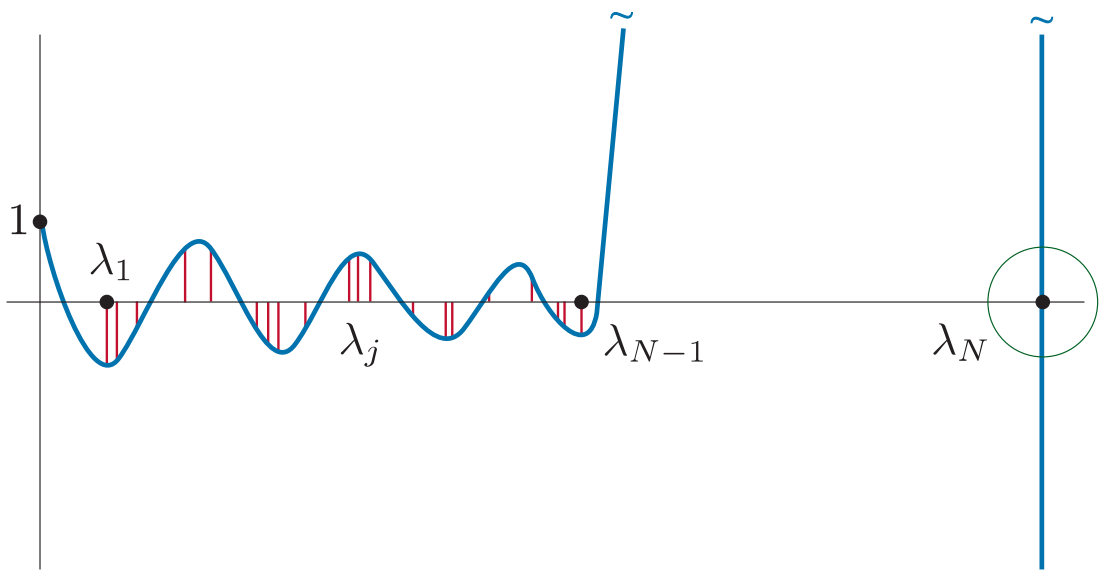

- Reduction of the condition number guarantees faster convergence of CG.
- The condition number bound based on Chebyshev polynomials

$$\frac{\|x - x_k\|_A}{\|x - x_0\|_A} \leq 2 \left(\frac{\sqrt{\kappa(\mathbf{B}^{-1}\mathbf{A})} - 1}{\sqrt{\kappa(\mathbf{B}^{-1}\mathbf{A})} + 1} \right)^k$$

  is usually descriptive for CG applied to symmetric positive definite (SPD) system with an SPD preconditioner.

Theoretical mathematical evidence proving incorrectness is persistently ignored and the misleading statements are repeatedly presented even in flagship journals.

3 The key concept for understanding: CG as the Gauss quadrature.

At any iteration step n, CG represents the matrix formulation of the n-point Gauss quadrature of the Riemann-Stieljes integral determined by $\mathbf{G}$ 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 $\omega^{(n)}(\lambda),\ n = 1, 2, \ldots$

3 CG (Lanczos) in finite precision arithmetic?

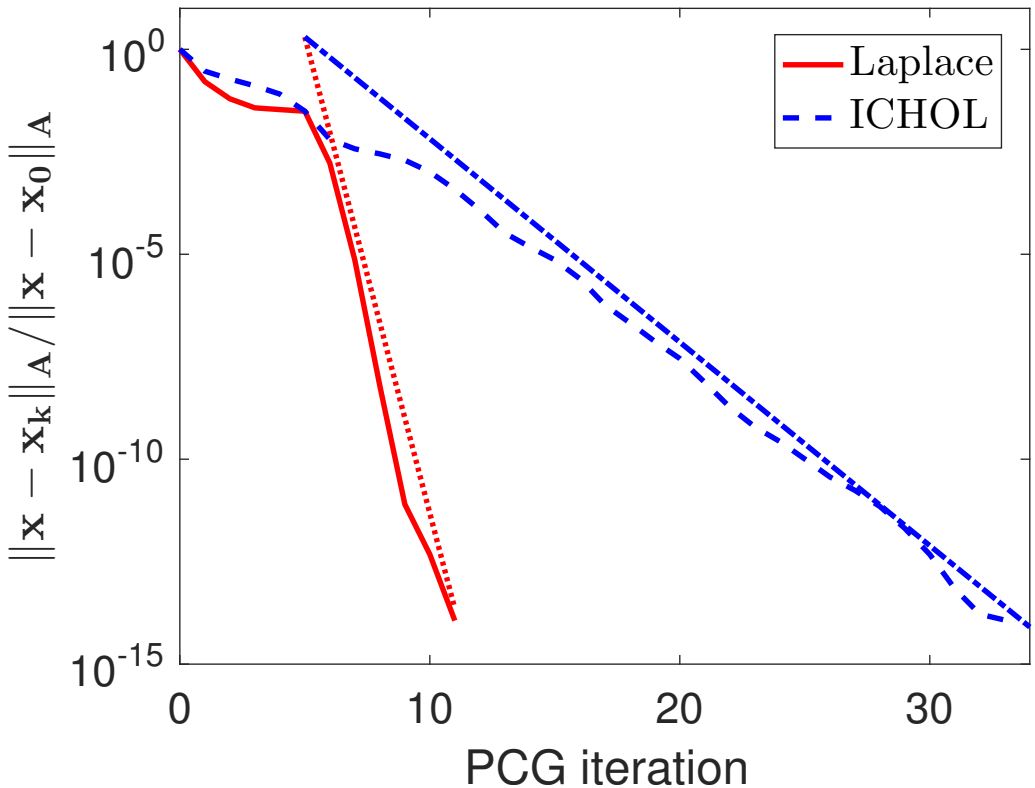
Rounding errors seemingly irreparably destroy the underlying mathematical structure that is based on orthogonality, and therefore the link with Gauss-Christoffel quadrature seems to be irreparably lost as well. However,

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 of the same weight.

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).

3 Back to the elliptic PDE example



- ICHOL PCG: $\kappa \approx 16$,
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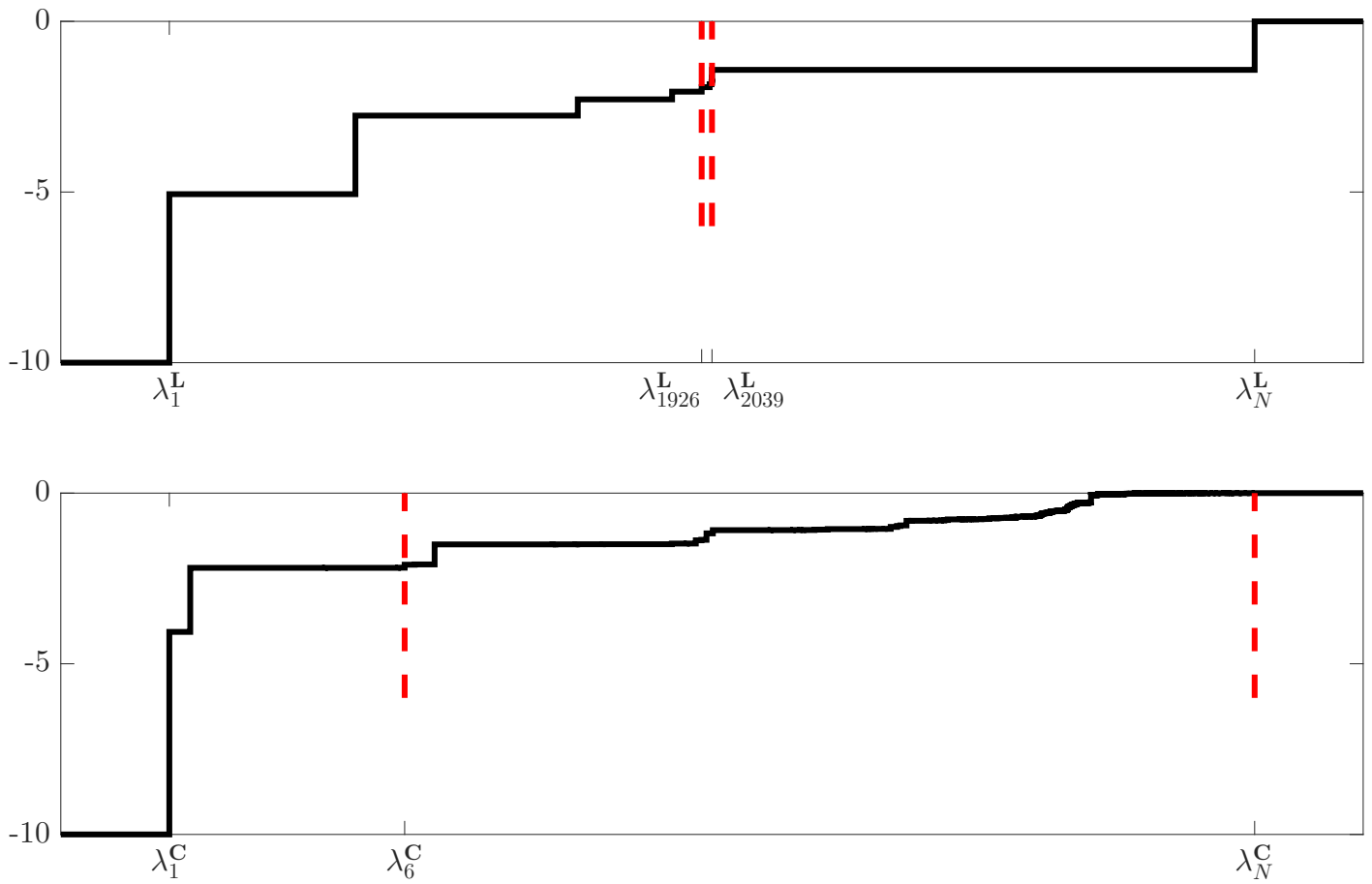
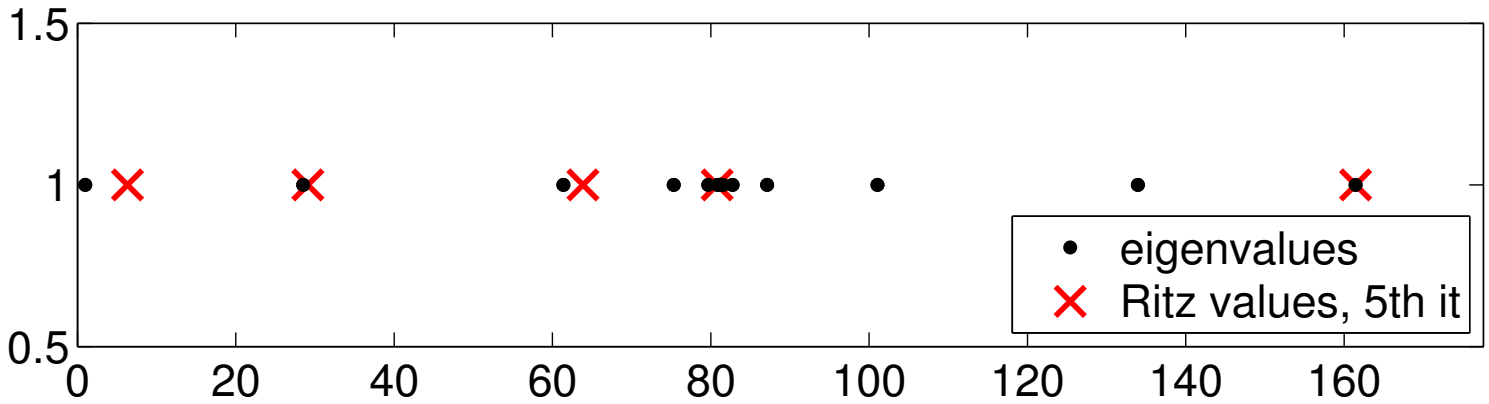
3 Various parts of the spectra and convergence behavior



The horizontal scales are different.

3 Ritz values at the 5th CG iteration - LAPL

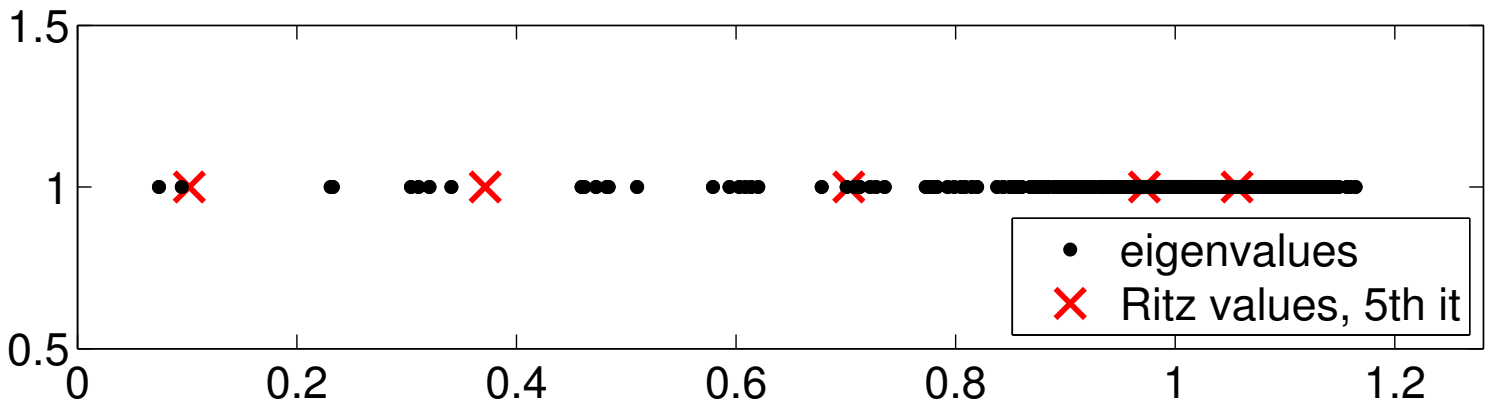


Index	1 – 1922	1923	1924	1925	1926
Eigenvalues	1	28.508	61.384	75.324	$\lambda^{\mathbf{L}}_{1926} = 79.699$
Total weight	9×10^{-6}	$\approx 10^{-3}$	$\approx 10^{-3}$	$\approx 10^{-3}$	$\approx 10^{-3}$

Index	1927 – 1930	1931 – 2039	2040 – 2047	2048 – 3969
Eigenvalues	80.875 – 81.222	$\lambda^{\mathbf{L}}_{2039} = 81.224$	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 ?

3 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	$\lambda_6^C = 0.311$	$0.321 - \lambda_{3969}^C = 1.1643$
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).

3 Observations and a question for further investigation

- Smaller condition number evidently does not guarantee faster CG convergence.
- Condition number bound is descriptive for the behavior of CG only under very particular circumstances. This conforms to a general mathematical principle: Highly nonlinear phenomena can be approximated by linear tools only locally.

3 Observations and a question for further investigation

- Smaller condition number evidently does not guarantee faster CG convergence.
- Condition number bound is descriptive for the behavior of CG only under very particular circumstances. This conforms to a general mathematical principle: Highly nonlinear phenomena can be approximated by linear tools only locally.

Spectrum of the preconditioned SPD matrix alone does not determine CG convergence behavior for a particular right-hand-side and initial approximation, but it offers much more than the trivialization of this n-dimensional nonlinear phenomenon using only condition number.

Can we can get cheap and accurate a priori information on the whole spectrum of the preconditioned matrices?

4 Stimulating work that formulated the open problem (2009)

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4 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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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

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

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.**

5 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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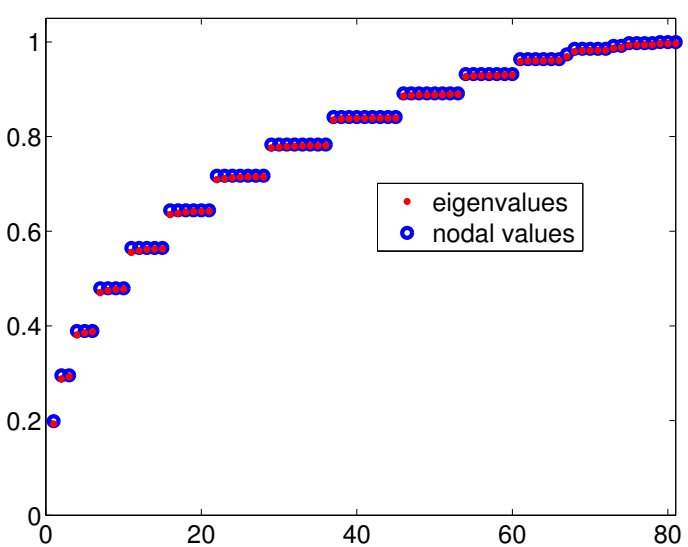
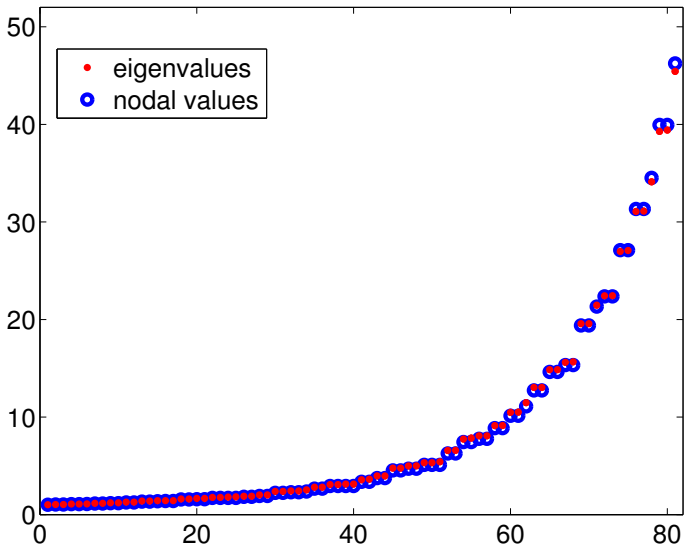
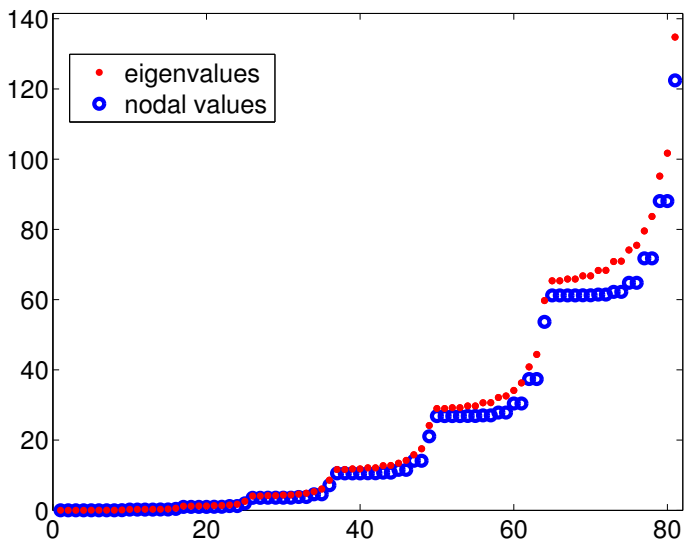
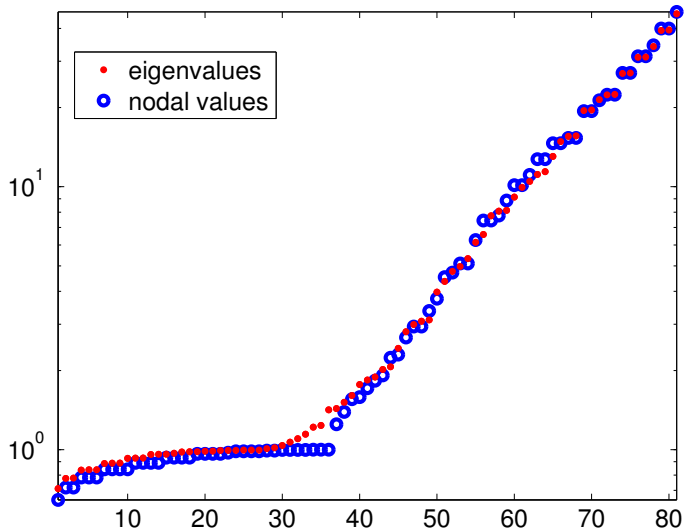
Proof:
Constructive perturbation argument and the Hall's theorem on bipartite graphs.
The operator $\mathcal{A}$ can be indefinite.

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









5 Important remark

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

The motivational problem given above:

- Almost 2000 eigenvalues are equal to 1.
- Almost 2000 eigenvalues are equal to 165.46.
- A few eigenvalues in between, for the supports where $k(x)$ is discontinuous. The associated eigenvalues are localized less accurately.

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

5 This opens other problems

- Generalizations to tensors?
- 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.

6 A priori approximation of the operator spectrum

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6 Infinite dimensional operator with symmetric tensor

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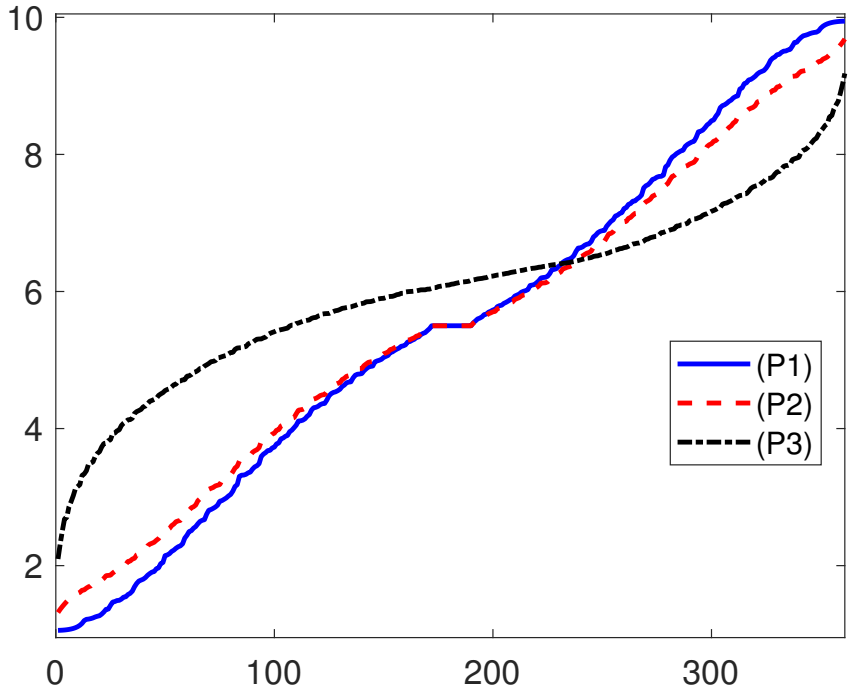
Assuming only that the symmetric tensor $K(x)$ is continuous **at least at a single point in** Ω and $\sup_{x\in\Omega} \kappa_1(x) < \inf_{x\in\Omega} \kappa_2(x)$, then the following closed interval belongs to the spectrum of $\mathcal{L}^{-1}\mathcal{A}$,

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

Analogous statement obviously holds with interchanging κ_1 and κ_2.

6 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 $\kappa_2(\overline{\Omega})$

Theorem (Spectrum of the preconditioned operator).

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

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

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

The spectrum of $\mathcal{B}^{-1}\mathcal{A}$ is defined as the complement of the resolvent set, i.e.,

$$\mathrm{sp}(\mathcal{B}^{-1}\mathcal{A}) = \{\lambda \in \mathbb{R}; \quad \lambda I - \mathcal{B}^{-1}\mathcal{A} \text{ does not have a bounded inverse}\}.$$

Theorem (Eigenvalues of the preconditioned matrices).

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.

Problem can be indefinite, preconditioner is SPD.

6 Remaining questions

- 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).

6 Remaining questions

- 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.

7 Convergence of the matrix eigenvalues towards the whole spectrum

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

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

7 Relationship between finite and infinite spectral information

For the specific cases we can get both lower and upper semicontinuity of the infinite dimensional spectrum. For the abstract setting used in the preceding Theorem we get only lower semicontinuity.

Here we approximate the whole spectrum of the bounded and continuously invertible operator $\mathcal{B}^{-1}\mathcal{A} : V \to V$ on the infinite dimensional Hilbert space, not the eigenvalues.

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Here we approximate the whole spectrum of the bounded and continuously invertible operator $\mathcal{B}^{-1}\mathcal{A} : V \to V$ on the infinite dimensional Hilbert space, not the eigenvalues.

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, Nielsen and S (2019) offers an explanation.

8 Spectral operator theory and PDE eigenvalue problems

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8 Compact PDE eigenvalue problem and approximating spectrum?

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- 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 whole infinite dimensional spectrum, including its continuous part, is relevant to the operator preconditioning, and, subsequently, to its algebraic realization.

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- 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 whole infinite dimensional spectrum, including its continuous part, is relevant to the operator preconditioning, and, subsequently, to its algebraic realization.
- This seems to be new and important point.

8 References used in this presentation

1. Málek, S, *Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs,* SIAM Spotlight Series, SIAM, Philadelphia, ISBN 978-1-611973-83-9, 2015,

2. Nielsen, Tveito and Hackbusch, *Preconditioning by inverting the Laplacian: An analysis of the eigenvalues* (IMA J. Numer. Anal., 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).

5. Gergelits, Nielsen and S, *Numerical approximation of the spectrum of self-adjoint operators in operator preconditioning* (Num. Alg., 2022).

6. Carson, Liesen and S, *70 years of the conjugate gradient method: the journey continues,* submitted, 2022, accessible via arxiv.

8 Remark

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).

8 Lanczos, Why Mathematics (1966)

"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."

8 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."

Radim, Ivo and Owe

Radim, Ivo and Owe

Thank you for all.