On Generalized Spectrum of Second Order Elliptic Differential Operators

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Based on a joint work with
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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 (sparse?) matrix problem

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

(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

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

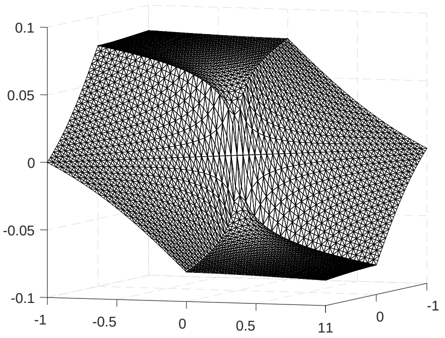
we get the approximation polynomial

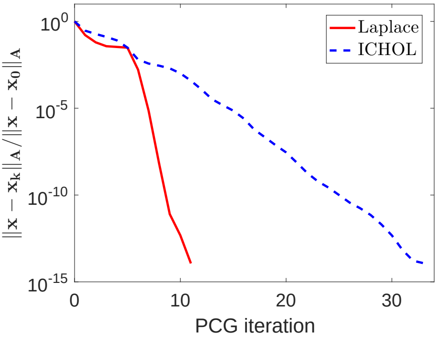
$$\varphi_n^{\mathrm{M}}(\lambda) = \;1 \;-\; \lambda\, p_{n-1}^{\mathrm{M}}(\lambda)\,,$$

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

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

Motivation: Class of elliptic PDEs, frequently used example





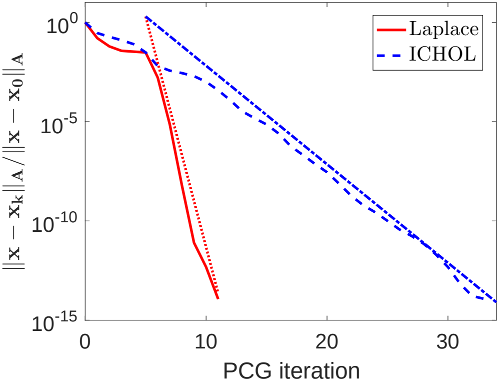
$$-\nabla \cdot (\, k(x)\, \nabla u\,) \;=\; 0\,,$$

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

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

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 et al. (2019), Localization of the eigenvalues of the discrete operator
4. Back to the infinite dimensional problem, tensor case
5. Outlook



Here we will not deal with the algorithmic and computational issues related to preconditioning. Therefore in the description of convergence we will consider a preconditioned system of equations.

Conjugate Gradient (CG) method for $Ax = b$ with A SPD (1952)

$r_0 = b - Ax_0,\ p_0 = r_0$. For $n = 1, \ldots, n_{\max}$:

$$\begin{aligned}
\alpha_{n-1} &= \frac{r_{n-1}^* r_{n-1}}{p_{n-1}^* A p_{n-1}} \\
x_n &= x_{n-1} + \alpha_{n-1} p_{n-1}\,, \quad \text{stop when the stopping criterion is satisfied} \\
r_n &= r_{n-1} - \alpha_{n-1} A p_{n-1} \\
\beta_n &= \frac{r_n^* r_n}{r_{n-1}^* r_{n-1}} \\
p_n &= r_n + \beta_n p_{n-1}
\end{aligned}$$

Here α_{n-1} ensures the minimization of the energy norm $\|x - x_n\|_A$ along the line

$$z(\alpha) = x_{n-1} + \alpha p_{n-1}\,.$$

1 Mathematical elegance of CG: orthogonality giving optimality

Provided that

$$p_i \perp_A p_j, \quad i \neq j,$$

the one-dimensional line minimizations at the individual steps 1 to n result in the n-dimensional minimization over the whole shifted Krylov subspace

$$x_0 + \mathcal{K}_n(A, r_0) \; = \; x_0 + \mathrm{span}\{p_0, p_1, \dots, p_{n-1}\}\,.$$

Indeed,

$$x - x_0 \; = \; \sum_{\ell=0}^{N-1} \alpha_\ell p_\ell \; = \; \sum_{\ell=0}^{n-1} \alpha_\ell p_\ell \; + \; x - x_n\,,$$

where

$$x - x_n \; \perp_A \; K_n(A, r_0)\,, \quad \text{or, equivalently,} \quad r_n \; \perp \; K_n(A, r_0)\,.$$

$$
\begin{aligned}
\|\mathbf{x}-\mathbf{x}_n\|_{\mathbf{A}}^2 &= \min_{\varphi\in\Pi_n} \|\varphi(\mathbf{A})(\mathbf{x}-\mathbf{x}_0)\|_{\mathbf{A}}^2 \\
&= \sum_{j=1}^{N} \lambda_j\, \zeta_j^2\, \varphi_n^{\mathrm{CG}}(\lambda_j)^2\,, \quad j=1,2,\ldots
\end{aligned}
$$

Here

$$
\varphi_n^{\mathrm{CG}}(\lambda) = \frac{(\lambda-\theta_1^{(n)})\cdots(\lambda-\theta_n^{(n)})}{(-1)^n\,\theta_1^{(n)}\cdots\theta_n^{(n)}}
$$

is determined by the eigenvalues of the orthogonally restricted operator, i.e., by the eigenvalues $\theta_1^{(n)},\ldots,\theta_n^{(n)}$ of $\mathbf{T}_n$ (Ritz values) .

Let $\omega^{(n)}(\lambda)$ be the distribution function determined by the n-node Gauss quadrature approximation of the Riemann-Stieltjes integral with the distribution function $\omega(\lambda)$ determined by the SPD matrix A and r_0. Then

$$\begin{tikzcd}
A,\ v_1 = r_0/\|r_0\| \arrow[r, leftrightarrow] \arrow[d] & \omega(\lambda),\ \int f(\lambda)\, d\omega(\lambda) \arrow[d] \\
\text{Hermitian Lanczos/CG} \arrow[d] & \text{Gauss-Christoffel quadrature} \arrow[d] \\
T_n,\ e_1 \arrow[r, leftrightarrow] & \omega^{(n)}(\lambda),\quad \sum_{j=1}^{n} \omega_j^{(n)} f(\theta_j^{(n)})
\end{tikzcd}$$

The quadrature nodes $\lambda_j^{(n)}$ are the eigenvalues $\theta_j^{(n)}$ of $\mathbf{T}_n$ and the weights $\omega_j^{(n)}$ are the squared first components of the associated normalized eigenvectors.

1 Size of the error is equal!

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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This has become the basis for CG error estimation; see Golub, 1994; and, e.g., the surveys in S and Tichý, 2002; Meurant and S, 2006; Golub and Meurant, 2010; Liesen and S, 2013.

1 Mathematical model of FP CG - perfidious clusters!

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

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

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

1 Adaptation as the main principle

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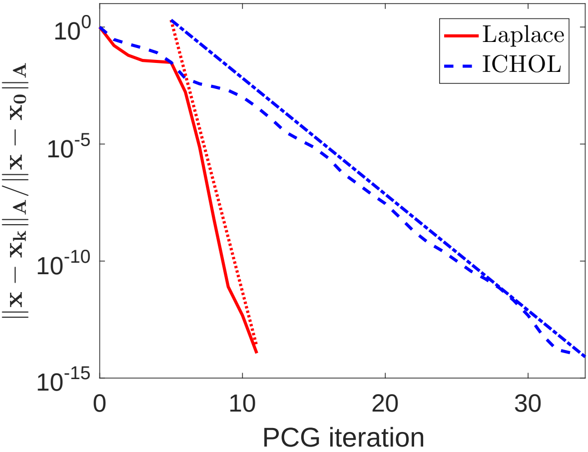
Now back to our motivating example.



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

- The CG optimality property

$$\|\mathbf{x}-\mathbf{x}_n\|_{\mathbf{A}} = \min_{\mathbf{z}\in\mathbf{x}_0+\mathcal{K}_n(\mathbf{A},\mathbf{r}_0)} \|\mathbf{x}-\mathbf{z}\|_{\mathbf{A}} = \min_{\varphi\in\Pi_n} \|\varphi(\mathbf{A})(\mathbf{x}-\mathbf{x}_0)\|_{\mathbf{A}}$$

yields in two derivation steps the (worst case) linear convergence bound valid and relevant for the Chebyshev method

$$\frac{\|\mathbf{x}-\mathbf{x}_n\|_{\mathbf{A}}}{\|\mathbf{x}-\mathbf{x}_0\|_{\mathbf{A}}} \le \min_{\varphi\in\Pi_n} \max_{1\le j\le N} |\varphi(\lambda_j)| \le \min_{p\in\Pi} \max_{\lambda\in[\lambda_1,\lambda_N]} |p(\lambda)|$$

$$\le 2\left(\frac{\sqrt{\kappa(\mathbf{A})}-1}{\sqrt{\kappa(\mathbf{A})}+1}\right)^n, \quad \kappa(\mathbf{A}) = \frac{\lambda_N}{\lambda_1}.$$

- The worst-case nonlinear bound is completely determined by the distribution of the eigenvalues of $\mathbf{A}$.

1 Linear "description" of the nonlinear CG method

- The CG optimality property

$$\|\mathbf{x}-\mathbf{x}_n\|_{\mathbf{A}} = \min_{\mathbf{z}\in\mathbf{x}_0+\mathcal{K}_n(\mathbf{A},\mathbf{r}_0)} \|\mathbf{x}-\mathbf{z}\|_{\mathbf{A}} = \min_{\varphi\in\Pi_n} \|\varphi(\mathbf{A})(\mathbf{x}-\mathbf{x}_0)\|_{\mathbf{A}}$$

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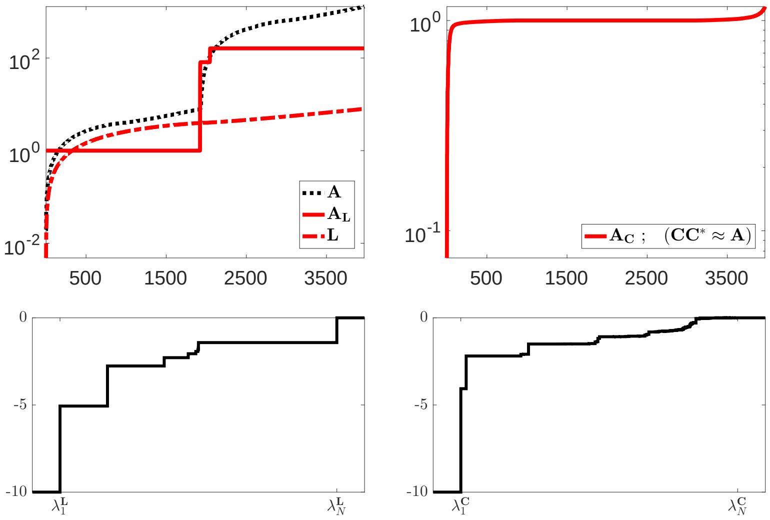
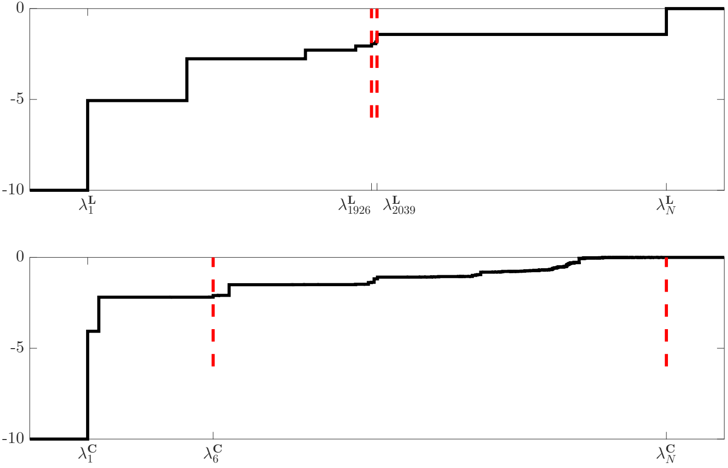
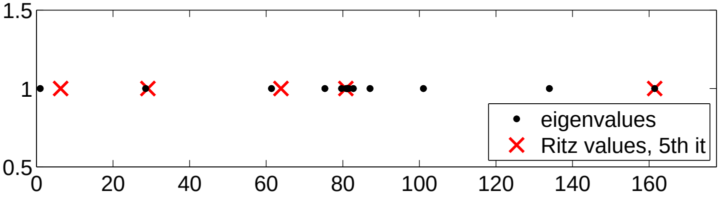


10^2
10^0
10^-2
500 1500 2500 3500
A
A_L
L
10^0
10^-1
A_C ; (CC* ≈ A)
0
-5
-10
λ_1^L
λ_N^L
λ_1^C
λ_N^C

1 Various parts of the spectra and convergence behavior



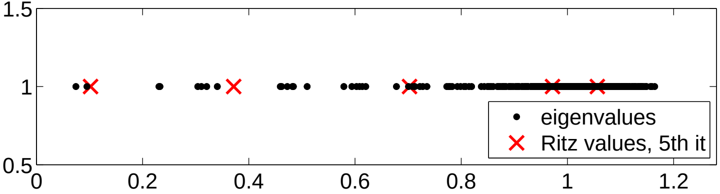
1 Ritz values at the 5th CG iteration - LAPL



Index	1 – 1922	1923	1924	1925	1926
Eigenvalues	1	28.508	61.384	75.324	$\lambda^{\mathbf{L}}_{1926} = 79.699$
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

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

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4. Back to the infinite dimensional problem, tensor case
5. Outlook

Consider the scalar real valued bounded and uniformly positive function $k(x) : \mathbb{R}^d \to \mathbb{R}$ and the generalized eigenvalue problem

$$\begin{aligned} \nabla \cdot (k(x)\nabla u) &= \lambda \Delta u \quad \text{in } \Omega \subset \mathbb{R}^d, \\ u = 0 & \qquad \text{on } \partial\Omega\,. \end{aligned}$$

Then

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

for all $x \in \Omega$ at which $k(x)$ is continuous, where

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

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

Consider a standard conforming FE discretization ($d = 1$, 2 or 3), which yields the generalized eigenvalue problem in the form

$$\mathbf{A}\mathbf{v} \;=\; \lambda\,\mathbf{L}\mathbf{v}.$$

Based on numerical observations, the authors conjecture that the spectrum of the discretized preconditioned algebraic operator

$$\mathbf{L}^{-1}\mathbf{A}$$

can be approximated by the nodal values of $k(x)$.

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Pairing the eigenvalues and the intervals $k(\mathcal{T}_j)\,,\ j = 1, \ldots, N$.

Let $0 < \lambda_1 \le \lambda_2 \le \ldots \le \lambda_N$ be the eigenvalues of $\mathbf{L}^{-1}\mathbf{A}$. Let $k(x)$ be 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

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

Pairing the eigenvalues and the nodal values

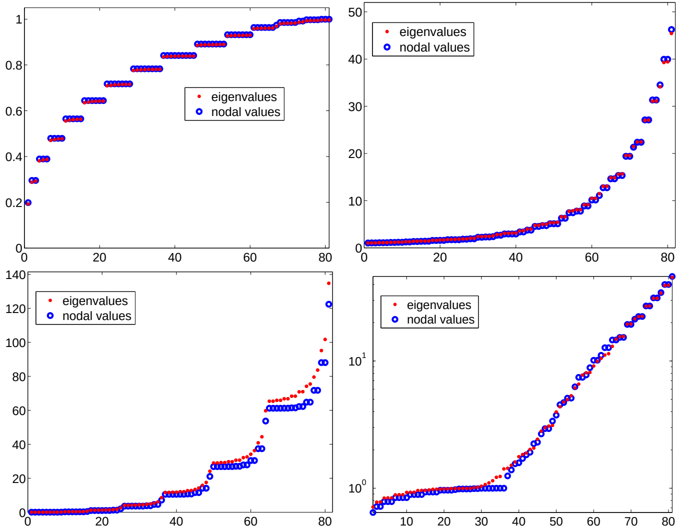
Consider any point $\hat{x}_j$ such that $\hat{x}_j \in \mathcal{T}_j$. Then the associated eigenvalue $\lambda_{\pi(j)}$ of the matrix $\mathbf{L}^{-1}\mathbf{A}$ satisfies

$$|\lambda_{\pi(j)} - k(\hat{x}_j)| \le \sup_{x \in \mathcal{T}_j} |k(x) - k(\hat{x}_j)|, \quad j = 1, \dots, N.$$

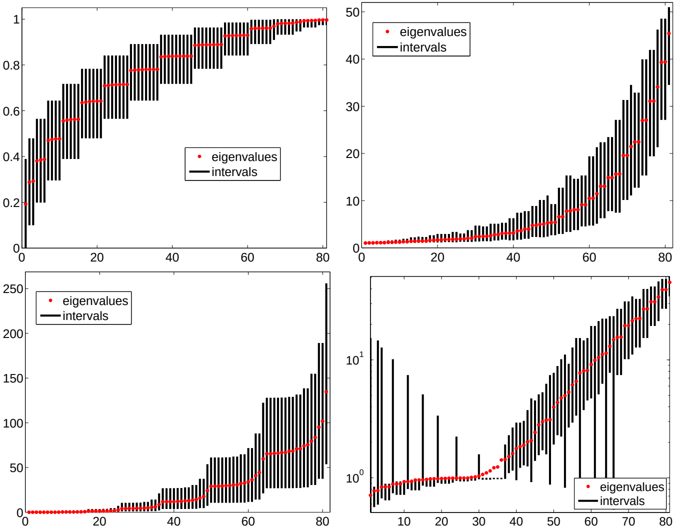
If, in addition, $k(x) \in \mathcal{C}^2(\mathcal{T}_j)$, then

$$\begin{aligned} |\lambda_{\pi(j)} - k(\hat{x}_j)| &\le \sup_{x \in \mathcal{T}_j} |k(x) - k(\hat{x}_j)| \\ &\le \hat{h}\,\|\nabla k(\hat{x}_j)\| + \tfrac{1}{2}\hat{h}^2 \sup_{x \in \mathcal{T}_j} \|D^2 k(x)\|, \quad j = 1, \dots, N, \end{aligned} \tag{1}$$

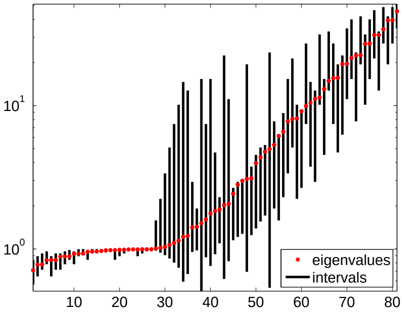
where $\hat{h} = \mathrm{diam}(\mathcal{T}_j)$ and $D^2 k(x)$ is the second order derivative of $k(x)$.

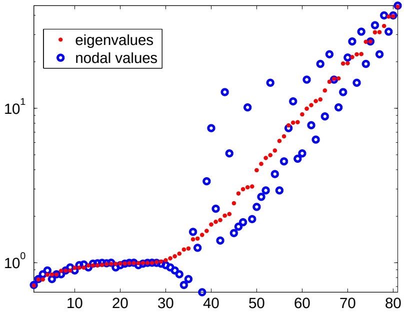

eigenvalues
nodal values
0
0.2
0.4
0.6
0.8
1
0
20
40
60
80
eigenvalues
nodal values
0
10
20
30
40
50
0
20
40
60
80
eigenvalues
nodal values
0
20
40
60
80
100
120
140
0
20
40
60
80
eigenvalues
nodal values
10^0
10^1
10
20
30
40
50
60
70
80

3 Intervals, pairing “defined” by increasing nodal values



3 Correct pairing illustrating proved results





Here we use discontinuous function $k(x, y)$, (problem P4 in the paper).

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Consider the generalized eigenvalue problem

$$\begin{aligned} \nabla \cdot (K \nabla u) &= \lambda \, \Delta u \quad \text{in } \Omega \,, \\ u &= 0 \qquad \text{on } \partial\Omega \,. \end{aligned}$$

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

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

where

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

Spectrum of the infinite dimensional preconditioned operator

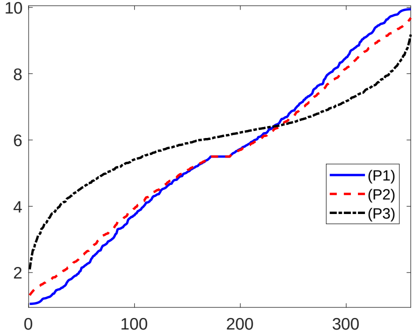
Consider an open and bounded Lipschitz domain $\Omega \subset \mathbb{R}^2$. Assume that the tensor $K(x, y)$ is symmetric and continuous throughout the closure $\overline{\Omega}$. Then the spectrum of the operator $\mathcal{L}^{-1}\mathcal{A}$ equals

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

where

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

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



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

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5 Work to be done

- Eigenvalues in the spectrum of the infinite dimensional operator?
- Discretized tensor case?
- Extension to 3D?
- Generalizations and preconditioning for practical problems?
-
-
-

Pre-conditioning?

Faber, Manteuffel and Parter, *On the theory of equivalent operators and application to the numerical solution of uniformly elliptic partial differential equations,* Advances in Applied Mathematics 11, 109–163 (1990):

"This work is motivated by the desire to construct a preconditioning strategy that yields bounds ..... independent of the mesh parameter h. ..... This leads to the conclusion that while equivalence [of operators] may be necessary to yield bounds independent of h, it is by no means sufficient to produce a good preconditioning strategy."

Pre-conditioning?

Faber, Manteuffel and Parter, *On the theory of equivalent operators and application to the numerical solution of uniformly elliptic partial differential equations,* Advances in Applied Mathematics 11, 109–163 (1990):

"This work is motivated by the desire to construct a preconditioning strategy that yields bounds ..... independent of the mesh parameter h. ..... This leads to the conclusion that while equivalence [of operators] may be necessary to yield bounds independent of h, it is by no means sufficient to produce a good preconditioning strategy."

Málek, S, *Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs,* SIAM Spotlights, SIAM (2015), Chapter 13:

"Here we do not argue against using condition numbers ... where appropriate. We argue against using them as general unquestioned tools which are considered fully descriptive ... as arguments closing the door for further investigation."

5 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."

5 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."

Thank you very much for your kind patience!