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Interpretation of the algebraic error and algebraic preconditioning as the transformation of the discretization basis

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Motivation

$$x \in V\,;\; \langle \mathcal{A}x, v\rangle = \langle b, v\rangle \quad \forall v \in V$$

finite-dimensional subspace $V_h \subset V$

$$x_h \in V_h\,;\; \langle \mathcal{A}x_h, v_h\rangle = \langle b, v_h\rangle \quad \forall v_h \in V_h$$

choice of the discretization basis Φ

Φ_1 Φ_2 Φ_3

$$\mathbf{A}_1\mathbf{x}_1 = \mathbf{b}_1 \qquad \mathbf{A}_2\mathbf{x}_2 = \mathbf{b}_2 \qquad \mathbf{A}_3\mathbf{x}_3 = \mathbf{b}_3$$

$$x_h = \Phi_1\,\mathbf{x}_1 \qquad x_h = \Phi_2\,\mathbf{x}_2 \qquad x_h = \Phi_3\,\mathbf{x}_3$$

Motivation

Question 1

Can we interpret algebraic preconditioning as transformation of the discretization basis functions?

Question 2

Can we interpret algebraic error as transformation of the discretization basis functions such that the computed non-Galerkin solution is the Galerkin solution with respect to the transformed basis?

Outline

1. **Setting and notation**
2. **Algebraic preconditioning and the transformation of the discretization basis**
3. **Interpretation of the algebraic error**

1. Basic notation

Let V be a real (infinite dimensional) Hilbert space with the inner product

$$(\cdot,\cdot)_V \,:\, V \times V \to \mathbf{R}\,,$$

$V^{\#}$ be the dual space of bounded linear functionals on V with the duality pairing

$$\langle\cdot,\cdot\rangle \,:\, V^{\#} \times V \to \mathbf{R}\,.$$

For each $f \in V^{\#}$ there exists a unique $\tau f \in V$ such that

$$\langle f, v\rangle = (\tau f, v)_V \quad \text{for all} \quad v \in V\,.$$

In this way the inner product $(\cdot,\cdot)_V$ determines the Riesz map

$$\tau \,:\, V^{\#} \to V\,.$$

1. Functional formulation

Consider a PDE problem described in the form of the functional equation

$$\mathcal{A}x = b\,, \quad \mathcal{A} : V \to V^{\#}, \quad x \in V, \quad b \in V^{\#} \tag{1}$$

where the linear, bounded, and coercive operator $\mathcal{A}$ is self-adjoint w.r.t. the duality pairing $\langle \cdot, \cdot \rangle$.

With the transformation using the Riesz map,

$$\tau\mathcal{A}x = \tau b\,, \qquad \tau\mathcal{A} \,:\, V \to V\,, \quad x \in V\,, \quad \tau b \in V\,,$$

which is called operator preconditioning.

Algebraic preconditioning and the transformation of the discretization basis

2. Related ideas and work

Operator preconditioning

[Klawonn (1995, 1996)]; [Arnold, Falk, and Winther (1997, 1997)]; [Steinbach and Wendland (1998)]; [McLean and Tran (1997)]; [Christiansen and Nédélec (2000, 2000)]; [Powell and Silvester (2003)]; [Elman, Silvester, and Wathen (2005, 2014)]; [Hiptmair (2006)]; [Axelsson and Karátson (2009)]; [Mardal and Winther (2011)]; [Kirby (2011)]; [Zulehner (2011)]; ...

CG in Hilbert spaces

[Hayes (1954)]; ...; [Glowinski (2003)]; [Axelsson and Karátson (2009)]; [Mardal and Winther (2011)]; [Günnel, Herzog and Sachs (2013)].

Hierarchical preconditioning, multilevel methods, domain decomposition with coarse components

[Yserentant (1985, 1986)], using the work of [Zienkiewicz et al. (1970)]; ...
[Axelsson and Vassilevski (1989)], the survey in [Vassilevski (2008)]; ...
[Jarošová, Klawonn and Rheinbach (2012)]; ...

2. Krylov manifolds in Hilbert spaces

Using the Riesz map, one can form for $x_0 \in V$, $r_0 \equiv b - \mathcal{A}x_0 \in V^{\#}$ the Krylov subspace

$$K_n \equiv \mathrm{span}\{\tau r_0, (\tau\mathcal{A})(\tau r_0), (\tau\mathcal{A})^2(\tau r_0), \ldots, (\tau\mathcal{A})^{n-1}(\tau r_0)\},$$

and approximate the solution $x = (\tau\mathcal{A})^{-1}\tau b$ constructing the approximations $x_n \in x_0 + K_n$ from the Krylov manifolds in V.

Looking for the approximate solution minimizing the energy leads to

$$\|x - x_n\|_a = \min_{z \in x_0 + K_n} \|x - z\|_a, \qquad \|z\|_a^2 \equiv \langle \mathcal{A}z, z\rangle,$$

which is equivalent to the Galerkin orthogonality condition

$$\langle b - \mathcal{A}x_n, w\rangle = 0 \qquad \text{for all } w \in K_n.$$

2. Preconditioned CG in Hilbert spaces

$$r_0 = b - \mathcal{A}x_0 \in V^{\#}, \quad p_0 = \tau r_0 \in V$$

$$x_n = x_{n-1} + \alpha_{n-1} p_{n-1} ,$$

$$\alpha_{n-1} = \frac{\langle r_{n-1}, \tau r_{n-1} \rangle}{\langle \mathcal{A}p_{n-1}, p_{n-1} \rangle} = \frac{(\tau r_{n-1}, \tau r_{n-1})_V}{(\tau \mathcal{A}p_{n-1}, p_{n-1})_V} ,$$

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

$$p_n = \tau r_n + \beta_n p_{n-1} ,$$

$$\beta_n = \frac{\langle r_n, \tau r_n \rangle}{\langle r_{n-1}, \tau r_{n-1} \rangle} = \frac{(\tau r_n, \tau r_n)_V}{(\tau r_{n-1}, \tau r_{n-1})_V} .$$

$\Phi = \{\phi_1, \ldots, \phi_N\}$

basis of the finite-dimensional subspace $V_h \subset V$,

$\Phi^\# = \{\phi_1^\#, \ldots, \phi_N^\#\}$

canonical basis of the dual $V_h^\#$, $\Phi^\# \Phi = \mathbf{I}$.

Using the coordinates in Φ and in $\Phi^\#$,

$$\begin{aligned}
\langle f, v\rangle &= \langle \Phi^\# \mathbf{f}, \Phi \mathbf{v}\rangle &&= \mathbf{v}^* \mathbf{f}\,,\\
(u, v)_{V_h} &= (\Phi \mathbf{u}, \Phi \mathbf{v})_{V_h} &&= \mathbf{v}^* \mathbf{M} \mathbf{u}\,,\\
\mathcal{A} u &= \mathcal{A} \Phi\, \mathbf{u} &&= \Phi^\# \mathbf{A} \mathbf{u}\,,\\
\tau f &= \tau \Phi^\# \mathbf{f} &&= \Phi\, \mathbf{M}^{-1}\, \mathbf{f}\,;
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{M} = [M_{ij}] &= [\,(\phi_j, \phi_i)_{V_h}\,]\,,\\
\mathbf{A} = [A_{ij}] &= [\,\langle \mathcal{A}\phi_j, \phi_i\rangle\,]\,, \qquad i, j = 1, \ldots, N\,.
\end{aligned}$$

Preconditioned CG

With $b = \Phi^{\#}\,\mathbf{b}\,, \quad x_n = \Phi\,\mathbf{x}_n\,,\ p_n = \Phi\,\mathbf{p}_n\,,\ r_n = \Phi^{\#}\,\mathbf{r}_n$ we get the standard preconditioned algebraic CG with the preconditioner $\mathbf{M}$.

Unpreconditioned CG is in this setting an oxymoron!

Unpreconditioned CG, i.e. $\mathbf{M} = \mathbf{I}$, corresponds to the basis Φ orthonormal w.r.t. the inner product $(\cdot,\cdot)_{V_h}$.

2. Orthogonalization of the discretization basis

Consider the decomposition $\mathbf{M} = \mathbf{L}\mathbf{L}^*$ and the transformed discretization basis $\Phi_t = \Phi\,(\mathbf{L}^*)^{-1}$ that is orthonormal w.r.t. $(\cdot,\cdot)_{V_h}$.

Then the matrix representation of CG in the Hilbert space V_h with the basis Φ_t gives the standard algebraic (unpreconditioned) CG applied to the preconditioned system

$$\mathbf{L}^{-1}\mathbf{A}(\mathbf{L}^*)^{-1}(\mathbf{L}^*\mathbf{x}) = \mathbf{L}^{-1}\mathbf{b}\,.$$

2. Interpretation of the algebraic preconditioning

For the algebraic preconditioning with $\widehat{\mathbf{L}}\widehat{\mathbf{L}}^* = \widehat{\mathbf{M}} \neq \mathbf{M}$, the (transformed) discretization basis $\widehat{\Phi} = \Phi\,(\widehat{\mathbf{L}}^*)^{-1}$ is not orthonormal w.r.t. $(\cdot,\cdot)_{V_h}$.

In order to obtain the interpretation of the algebraic preconditioning $\widehat{\mathbf{M}}$ as the transformation of the basis $\Phi \to \widehat{\Phi}$, we have to change also the inner product in V_h:

$$(u,v)_{V_h} = (\Phi\,\mathbf{u}, \Phi\,\mathbf{v})_{V_h} = \mathbf{v}^*\mathbf{M}\mathbf{u}\,,$$

has to be replaced by

$$(u,v)_{\mathrm{new},V_h} = (\widehat{\Phi}\,\widehat{\mathbf{u}}, \widehat{\Phi}\,\widehat{\mathbf{v}})_{\mathrm{new},V_h} \equiv \widehat{\mathbf{v}}^*\widehat{\mathbf{u}} = \mathbf{v}^*\widehat{\mathbf{M}}\mathbf{u}\,.$$

2. Observations

Algebraic preconditioning associated with the operator preconditioning is equivalent to the orthogonalization of the discretization basis in the given finite-dimensional Hilbert space V_h .

Algebraic preconditioning can be interpreted as transformation of the discretization basis and, at the same time, transformation of the inner product in V_h such that the transformed basis $\widehat{\Phi}$ is orthonormal with respect to the transformed inner product.

Interpretation of the algebraic error

3. Algebraic backward error

Let $\mathbf{x}$ solves the discretized algebraic system

$$\mathbf{A}\mathbf{x} = \mathbf{b}\,, \qquad A_{ij} = \langle \mathcal{A}\phi_j, \phi_i \rangle\,, \quad b_i = \langle b, \phi_i \rangle$$

and let the algebraic vector $\widehat{\mathbf{x}}$ which approximates $\mathbf{x}$ solves the perturbed system

$$(\mathbf{A} + \mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b} + \mathbf{f}\,.$$

Our aim is to interpret the perturbations $\mathbf{E}, \mathbf{f}$ as transformation of the discretization bases.

We will consider possibly different transformation of the discretization (search) and the test bases

$$\begin{aligned} \widehat{\Phi} &= \Phi\,(\mathbf{I} + \mathbf{D})\,, \\ \widetilde{\Phi} &= \Phi\,(\mathbf{I} + \mathbf{G})\,. \end{aligned}$$

3. Transformation of the discretization bases

Let the Galerkin solution $x_h = \Phi\,\mathbf{x}$ of the discretized formulation

$$\langle \mathcal{A}x_h, \phi_i \rangle \;=\; \langle b, \phi_i \rangle, \quad i = 1, \ldots, N$$

can be expressed as the Galerkin solution $x_h = \widehat{\Phi}\,\widehat{\mathbf{x}} = \Phi\,(\mathbf{I} + \mathbf{D})\,\widehat{\mathbf{x}}$ of the formulation

$$\langle \mathcal{A}x_h, \widetilde{\phi}_i \rangle \;=\; \langle b, \widetilde{\phi}_i \rangle, \quad i = 1, \ldots, N\,.$$

Discretization via the transformed basis functions $\widehat{\Phi}$ and the test functions $\widetilde{\Phi}$ results in the linear algebraic system

$$\overline{\mathbf{A}}\widehat{\mathbf{x}} = \overline{\mathbf{b}}\,, \qquad \overline{A}_{ij} \;=\; \langle \mathcal{A}\widehat{\phi}_j, \widetilde{\phi}_i \rangle\,, \quad \overline{b}_i = \langle b, \widetilde{\phi}_i \rangle\,,$$

where $\overline{\mathbf{A}} = (\mathbf{I} + \mathbf{G})^T\mathbf{A}\,(\mathbf{I} + \mathbf{D})$ and $\overline{\mathbf{b}} = (\mathbf{I} + \mathbf{G})^T\mathbf{b}\,.$

3. Interpretation of the algebraic error

The algebraic vector $\widehat{\mathbf{x}}$ which approximates $\mathbf{x}$ solves exactly the algebraic system determined by the Galerkin discretization of the infinite dimensional problem.

Interpreting the perturbations in

$$(\mathbf{A} + \mathbf{E})\, \widehat{\mathbf{x}} = \mathbf{b} + \mathbf{f}$$

as transformation of the discretization bases gives

$$\begin{aligned} \mathbf{A} + \mathbf{E} &= (\mathbf{I} + \mathbf{G})^T \mathbf{A}\, (\mathbf{I} + \mathbf{D})\,, \\ \mathbf{b} + \mathbf{f} &= (\mathbf{I} + \mathbf{G})^T \mathbf{b}\,. \end{aligned}$$

3. Three classes of backward errors

Perturbed algebraic system

$$(\mathbf{A} + \mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b} + \mathbf{f}\,.$$

1. $\mathbf{E} \neq 0\,,\ \mathbf{f} \neq 0\,,$
2. $\mathbf{A} + \mathbf{E}$ is symmetic positive definite,
3. $\mathbf{f} = 0\,.$

3. General case ($\mathbf{E} \neq 0$, $\mathbf{f} \neq 0$)

Given perturbations $\mathbf{E}, \mathbf{f}$ satisfying $(\mathbf{A}+\mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b}+\mathbf{f}$, there are infinitely many couples of matrices $\mathbf{D}, \mathbf{G}$ satisfying

$$\begin{aligned} \mathbf{A}+\mathbf{E} &= (\mathbf{I}+\mathbf{G})^T \mathbf{A}\,(\mathbf{I}+\mathbf{D})\,, \\ \mathbf{b}+\mathbf{f} &= (\mathbf{I}+\mathbf{G})^T \mathbf{b}\,. \end{aligned}$$

Pick any $\mathbf{G}$ such that $\mathbf{G}^T\mathbf{b} = \mathbf{f}$ and $(\mathbf{I}+\mathbf{G})$ is nonsingular. Set

$$\mathbf{D} = \mathbf{A}^{-1}\left(\mathbf{I}+\mathbf{G}^T\right)^{-1}\left(\mathbf{E}-\mathbf{G}^T\mathbf{A}\right).$$

Outlook: The optimal choice of $\mathbf{D}$, $\mathbf{G}$?

3. Symmetric case ($\mathbf{A} + \mathbf{E}$ is SPD)

In order to preserve the symmetry take $\mathbf{D} = \mathbf{G}$. Then

$$\mathbf{A} + \mathbf{E} = (\mathbf{I} + \mathbf{D})^T \mathbf{A} (\mathbf{I} + \mathbf{D}), \tag{2}$$

$$\mathbf{b} + \mathbf{f} = (\mathbf{I} + \mathbf{D})^T \mathbf{b}. \tag{3}$$

$\mathbf{D}$ satisfies (2) if and only if

$$\mathbf{I} + \mathbf{D} = \mathbf{A}^{-1/2} \mathbf{U} (\mathbf{A} + \mathbf{E})^{1/2}, \quad \mathbf{U} \text{ is an orthogonal matrix.}$$

From (3) we obtain the condition

$$\mathbf{b}^T \mathbf{x} = (\mathbf{b} + \mathbf{f})^T \widehat{\mathbf{x}}, \quad \text{or, equivalently,} \quad \|\mathbf{x}\|_{\mathbf{A}} = \|\widehat{\mathbf{x}}\|_{\mathbf{A}+\mathbf{E}},$$

which in general does not hold.

3. Backward error with $\mathbf{f} = 0$

When $\mathbf{f} = 0$, it is natural to set $\mathbf{G} = 0$, i.e. to consider original test functions. This case was considered in [Gratton, Jiránek, and Vasseur (2013)]; [P., Liesen, Strakoš (2014)].

From $\mathbf{A} + \mathbf{E} = \mathbf{A}\,(\mathbf{I} + \mathbf{D})$ we have $\mathbf{A}\mathbf{D} = \mathbf{E}$ and $\mathbf{D} = \mathbf{A}^{-1}\mathbf{E}$.

Loss of locality: the transformed basis $\widehat{\Phi} = \Phi\,(\mathbf{I} + \mathbf{D})$ has global support ($\mathbf{D}$ is dense)!

3. Loss of locality

Illustration on 1D Poisson model problem, using two perturbations in

$$(\mathbf{A} + \mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b}\,.$$

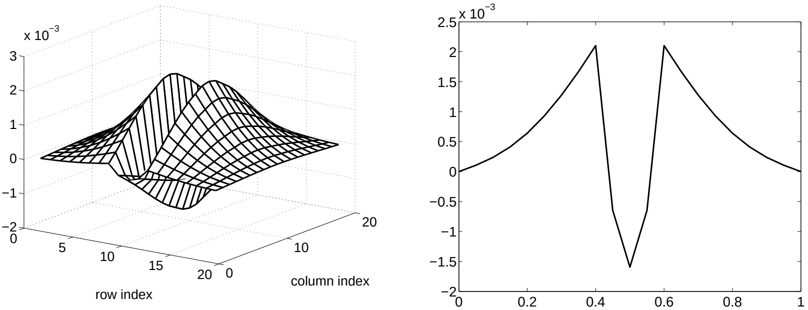
- $\mathbf{E} = \dfrac{(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}})\,\widehat{\mathbf{x}}^T}{\|\widehat{\mathbf{x}}\|_2^2}$, then $\mathbf{D} = \mathbf{A}^{-1}\mathbf{E} = \dfrac{(\mathbf{x} - \widehat{\mathbf{x}})\,\widehat{\mathbf{x}}^T}{\|\widehat{\mathbf{x}}\|_2^2}$,

- symmetric perturbation $\mathbf{E}_{\text{sym}}$ with the minimal Frobenius norm

$$\mathbf{E}_{\text{sym}} = \arg\min \left\{ \|\mathbf{E}\|_F \quad | \quad \mathbf{E} = \mathbf{E}^T\,,\ (\mathbf{A} + \mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b} \right\} ;$$

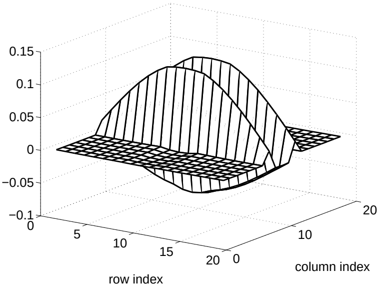
see [Bunch, Demmel, and van Loan (1989)].

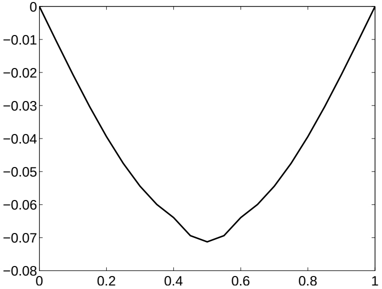
3. Transformed basis



MATLAB `surf` plot of the transformation matrix $\mathbf{D} = \mathbf{A}^{-1}\mathbf{E}$ (left) and the difference $\widehat{\phi}_j - \phi_j$ (right).

3. Transformed basis for symmetric perturbation matrix





MATLAB `surf` plot of the transformation matrix $\mathbf{D} = \mathbf{A}^{-1}\mathbf{E}_{\text{sym}}$ (left) and the difference $\widehat{\phi}_j - \phi_j$ (right).

Please note that $\|\mathbf{A}^{-1}\mathbf{E}_{\text{sym}}\| \gg \|\mathbf{A}^{-1}\mathbf{E}\|$!

References

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Thank you for your attention!