Backward error analysis and stopping criteria for Krylov space method

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Outline

- Backward error and norms
- Krylov methods and stopping criteria
- Elliptic problems
- Conclusions and future work

Linear systems

$$\mathbf{A}\mathbf{u} = \mathbf{b}$$

$\mathbf{A} \in \mathbb{R}^{N \times N}$ positive definite

Linear systems: variational framework

- Find $\mathbf{u} \in \mathcal{H}$ such that for all $\mathbf{v} \in \mathcal{H}$

$$a(\mathbf{u}, \mathbf{v}) = L(\mathbf{v}) \qquad (L(\cdot) \in \mathcal{H}' \text{ dual space of } \mathcal{H})$$

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- Existence and uniqueness: $\forall \mathbf{v}, \mathbf{w} \in \mathcal{H}$

$$\begin{aligned} a(\mathbf{w}, \mathbf{v}) &\leq C_1 \|\mathbf{w}\|_{\mathcal{H}} \|\mathbf{v}\|_{\mathcal{H}} \\ \sup_{\mathbf{w} \in \mathcal{H} \setminus \{0\}} \frac{a(\mathbf{w}, \mathbf{v})}{\|\mathbf{w}\|_{\mathcal{H}}} &\geq C_2 \|\mathbf{v}\|_{\mathcal{H}} \end{aligned}$$

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- $\mathcal{H} = (\mathbf{R}^N, || \cdot ||_{\mathbf{H}})$ and $\mathcal{H}' = (\mathbf{R}^N, || \cdot ||_{\mathbf{H}^{-1}})$ $\mathbf{H}$ SPD

Backward error

We have the following equivalence:

$$\left.\begin{array}{l}\exists b \in \mathcal{BL}(\mathcal{H}), \exists \delta L \in \mathcal{H}' \text{ such that:} \\ a(\tilde{\mathbf{u}}, \mathbf{v}) + b(\tilde{\mathbf{u}}, \mathbf{v}) = (L + \delta L)(\mathbf{v}), \\ \forall \mathbf{v} \in \mathcal{H}, \text{ and} \\ \|b(\cdot,\cdot)\|_{\mathcal{BL}(\mathcal{H})} \leq \alpha, \|\delta L\|_{\mathcal{H}'} \leq \beta \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} \|\rho_{\tilde{\mathbf{u}}}\|_{\mathcal{H}'} \leq \alpha \|\tilde{\mathbf{u}}\|_{\mathcal{H}} + \beta \\ \text{where } \rho_{\tilde{\mathbf{u}}} \in \mathcal{H}' \text{ is defined by} \\ \langle \rho_{\tilde{\mathbf{u}}}, \mathbf{v} \rangle_{\mathcal{H}',\mathcal{H}} = a(\tilde{\mathbf{u}}, \mathbf{v}) - L(\mathbf{v}), \\ \forall \mathbf{v} \in \mathcal{H} \end{array}\right.$$

Rigak and Gaches (1967), A., Noulard, and Russo (2001)

The symmetric case: conjugate gradient method

A symmetric positive definite

$\mathcal{H} = (\mathbf{R}^N, ||\cdot||_{\mathbf{A}})$ and $\mathcal{H}' = (\mathbf{R}^N, ||\cdot||_{\mathbf{A}^{-1}})$

At each step k the conjugate gradient method minimizes the energy norm of the error $\delta\mathbf{u}^{(k)} = \mathbf{u} - \mathbf{u}^{(k)}$ on a Krylov space $\mathbf{u}^{(0)} + \mathcal{K}_k$:

$$\min_{\mathbf{u}^{(k)} \in \, \mathbf{u}^{(0)} + \mathcal{K}_k} \|\delta\mathbf{u}^{(k)}\|^2_{\mathbf{A}}$$

$$\|\delta\mathbf{u}^{(k)}\|_{\mathbf{A}} = \|\rho_{\mathbf{u}^{(k)}}\|_{\mathcal{H}} = \|r^{(k)}\|_{\mathbf{A}^{-1}}$$

$$r^{(k)} = \mathbf{b} - \mathbf{A}\mathbf{u}^{(k)}$$

The symmetric case: stopping criteria

- Classic Criterion:

$$\text{IF } \|\mathbf{A}\mathbf{u}^{(k)} - \mathbf{b}\|_2 \le \sqrt{\varepsilon}\|\mathbf{b}\|_2 \text{ THEN STOP },$$

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with $\eta < 1$ an a-priori threshold fixed by the user.

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$$\text{IF } \|\mathbf{Au}^{(k)} - \mathbf{b}\|_2 \leq \sqrt{\varepsilon}\|\mathbf{b}\|_2 \text{ THEN STOP },$$

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with $\eta < 1$ an a-priori threshold fixed by the user. The choice of η will depend on the properties of the problem that we want to solve, and, in the practical cases, η can be frequently much larger than ε , the roundoff unit of the computer finite precision arithmetic.

The symmetric case: stopping criteria cont.

$$\|\mathbf{A}\mathbf{u}^{(k)} - \mathbf{b}\|_{\mathbf{A}^{-1}} \ ?$$

The symmetric case: stopping criteria cont.

$$\|\mathbf{A}\mathbf{u}^{(k)} - \mathbf{b}\|_{\mathbf{A}^{-1}} \quad ?$$

$$\|\mathbf{b}\|_{A^{-1}} \quad ?$$

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  - Gauss-Lobatto and Gauss-Radau. They compute lower and upper bounds using the extremes eigenvalues of $\mathbf{A}$.

The symmetric case: Hestenes-Stiefel rule

During the conjugate gradient iterates, we compute the scalar α_k and the conjugate vectors $\mathbf{p}^{(k)}$ ($\mathbf{p}^{(j)T}\mathbf{A}\mathbf{p}^{(i)} = 0,\ j \neq i$) and the residuals $r^{(k)}$. Thus,

$$\mathbf{u} = \sum_{j=1}^{\mathbf{N}} \alpha_j \mathbf{p}^{(j)}$$

and

$$\|\delta\mathbf{u}^{(k)}\|_{\mathbf{A}}^2 = \|\mathbf{A}\mathbf{u}^{(k)} - \mathbf{b}\|_{\mathbf{A}^{-1}}^2 = e_{\mathbf{A}}^2 = \sum_{j=k+1}^{\mathbf{N}} \alpha_j r^{(j)T} r^{(j)}$$

The symmetric case: Hestenes-Stiefel rule

Under the assumption that $e_{\mathbf{A}}^{(k+d)} << e_{\mathbf{A}}^{(k)}$, where the integer d denotes a suitable delay, the Hestenes and Stiefel estimate ξ_k will be

$$\xi_k = \sum_{j=k+1}^{k+d} \alpha_j r^{(j)T} r^{(j)}.$$

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The choice of a value for d depends on preconditioner and ill-conditioning.

$\mathbf{b}^T\mathbf{A}^{-1}\mathbf{b}$

From

$$r^{(k)T}\mathbf{v} = 0, \qquad \forall \mathbf{v} \in \mathcal{K}_k,$$

we prove

$$\mathbf{b}^T\mathbf{A}^{-1}\mathbf{b} = \mathbf{u}^T\mathbf{A}\mathbf{u} \geq \mathbf{u}^{(k)T}r^{(0)} + \mathbf{b}^T\mathbf{u}^{(0)},$$

(the right-hand side will converge monotonically to $\|\mathbf{u}\|^2_{\mathbf{A}}$).
Therefore, we use the following stopping criterion

$$\text{IF } \xi_k \leq \eta^2(\mathbf{u}^{(k)T}r^{(0)} + \mathbf{b}^T\mathbf{u}^{(0)}) \text{ THEN STOP .}$$

Preconditioning

The dual norm of the preconditioned residual is equal to the dual norm of the original residual.

Continuous problem

$$a(u,v) = \int_\Omega \mathfrak{K}(x)\nabla u \cdot \nabla v d\mathbf{x}, \quad \forall u,v \in H_0^1(\Omega)$$

$\forall u, v \in H_0^1(\Omega)$, $\exists \gamma \in \mathbf{R}_+$ and $\exists M \in \mathbf{R}_+$ such that

$$\begin{aligned} \gamma ||u||^2_{1,\Omega} \leq \quad & a(u,u) \\ & a(u,v) \quad \leq M||u||_{1,\Omega}||v||_{1,\Omega} \ , \end{aligned}$$

$L(v) = \int_\Omega f v d\mathbf{x}$, $L(v) \in H^{-1}(\Omega)$.

$$(P) \begin{cases} \text{Find } u \in H_0^1(\Omega) \text{ such that} \\ a(u,v) = L(v), \ \ \forall v \in H_0^1(\Omega), \end{cases}$$

has a unique solution.

Finite-element approximation

- Weak formulation

$$\begin{cases} \text{Find } u_h \in \mathcal{H}_h \text{ such that} \\ a_h(u_h, v_h) = L_h(v_h), \quad \forall v_h \in \mathcal{H}_h, \end{cases}$$

Finite element methods choose $\mathcal{H}_h$ to be a space of functions v_h defined on a subdivision Ω_h of Ω into simplices T of diameter h_T ; h denotes a piecewise constant function defined on Ω_h via $h|_T = h_T$.

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- Existence and uniqueness: $\mathcal{H}_h \subset \mathcal{H} = H_0^1(\Omega)$.
- Error Estimate: $\|u - u_h\|_{\mathcal{H}} \leq C(h)$

Finite-element framework

Solve

$$\mathbf{A}\mathbf{u}_h = \mathbf{b}$$

given

$$\sup_{\mathbf{w}\in\mathbb{R}^n\backslash\{\mathbf{0}\}} \sup_{\mathbf{v}\in\mathbb{R}^n\backslash\{\mathbf{0}\}} \frac{\mathbf{w}^t\mathbf{A}\mathbf{v}}{\|\mathbf{v}\|_{\mathbf{H}}\|\mathbf{w}\|_{\mathbf{H}}} \leq C_1 \qquad \text{(sup-sup)}$$

$$\inf_{\mathbf{w}\in\mathbb{R}^n\backslash\{\mathbf{0}\}} \sup_{\mathbf{v}\in\mathbb{R}^n\backslash\{\mathbf{0}\}} \frac{\mathbf{w}^t\mathbf{A}\mathbf{v}}{\|\mathbf{v}\|_{\mathbf{H}}\|\mathbf{w}\|_{\mathbf{H}}} \geq C_2 \qquad \text{(inf-sup)}$$

Note: $\|v_h\|_{\mathcal{H}_h} = \|\mathbf{v}\|_{\mathbf{H}}$.

Finite-element framework

Finally, assuming $h < 1$ and $t > 0$, and choosing $\eta = \mathcal{O}(h)$, we have

$$\|u - u_h^{(k)}\|_{\mathcal{H}} \leq C^*(h^t)\|u\|_{\mathcal{H}} + 2\|u - u_h\|_{\mathcal{H}} \leq C(h).$$

where

- $u(\mathbf{x})$ is the exact solution of the variational problem,
- $u_h(\mathbf{x})$ is the exact solution of the approximate problem,
- $u_h^{(k)}(\mathbf{x}) = \sum_{i=1}^{N} \mathbf{u}_h^{(k)} \phi_i(\mathbf{x})$ is the approximate solution at step k. ($\phi_i(\mathbf{x})$ are the basis functions)

Test problems

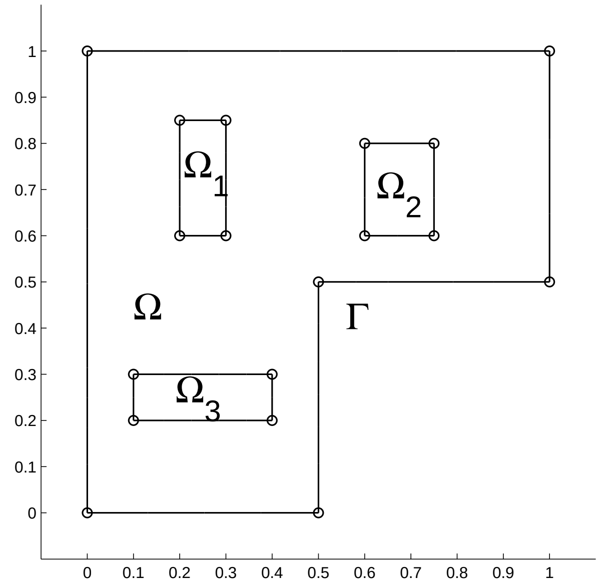
Problem 1

$$\mathfrak{K}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \Omega \setminus \{\Omega_1 \cup \Omega_2 \cup \Omega_3\}, \\ 10^{-6} & \mathbf{x} \in \Omega_1, \\ 10^{-4} & \mathbf{x} \in \Omega_2, \\ 10^{-2} & \mathbf{x} \in \Omega_3. \end{cases}$$

Problem 2

$$\mathfrak{K}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \Omega \setminus \{\Omega_1 \cup \Omega_2 \cup \Omega_3\}, \\ 10^{6} & \mathbf{x} \in \Omega_1, \\ 10^{4} & \mathbf{x} \in \Omega_2, \\ 10^{2} & \mathbf{x} \in \Omega_3. \end{cases}$$

$$L(v) = \int_\Omega 10 v d\mathbf{x}, \qquad \forall v \in H_0^1(\Omega)$$



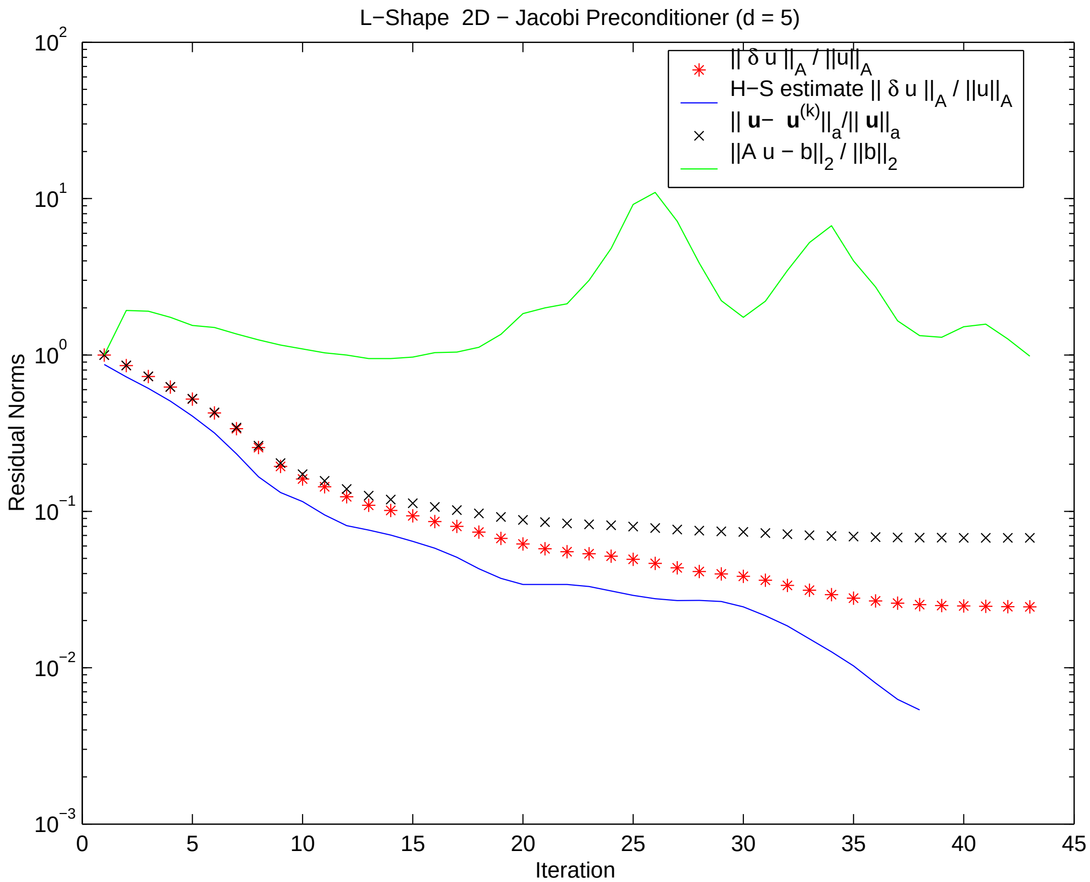
Preconditioners: estimates for $\kappa(\mathbf{M}^{-1}\mathbf{A})$

M	Problem 1	Problem 2
I	$3.6\ 10^8$	$1.8\ 10^{10}$
Jacobi	$2.4\ 10^4$	$1.5\ 10^9$
Inc. Cholesky(0)	$7.2\ 10^3$	$4.3\ 10^8$

$\eta^2 = 3.44.30510^{-5}$ and $\mathbf{N} = 29619.$

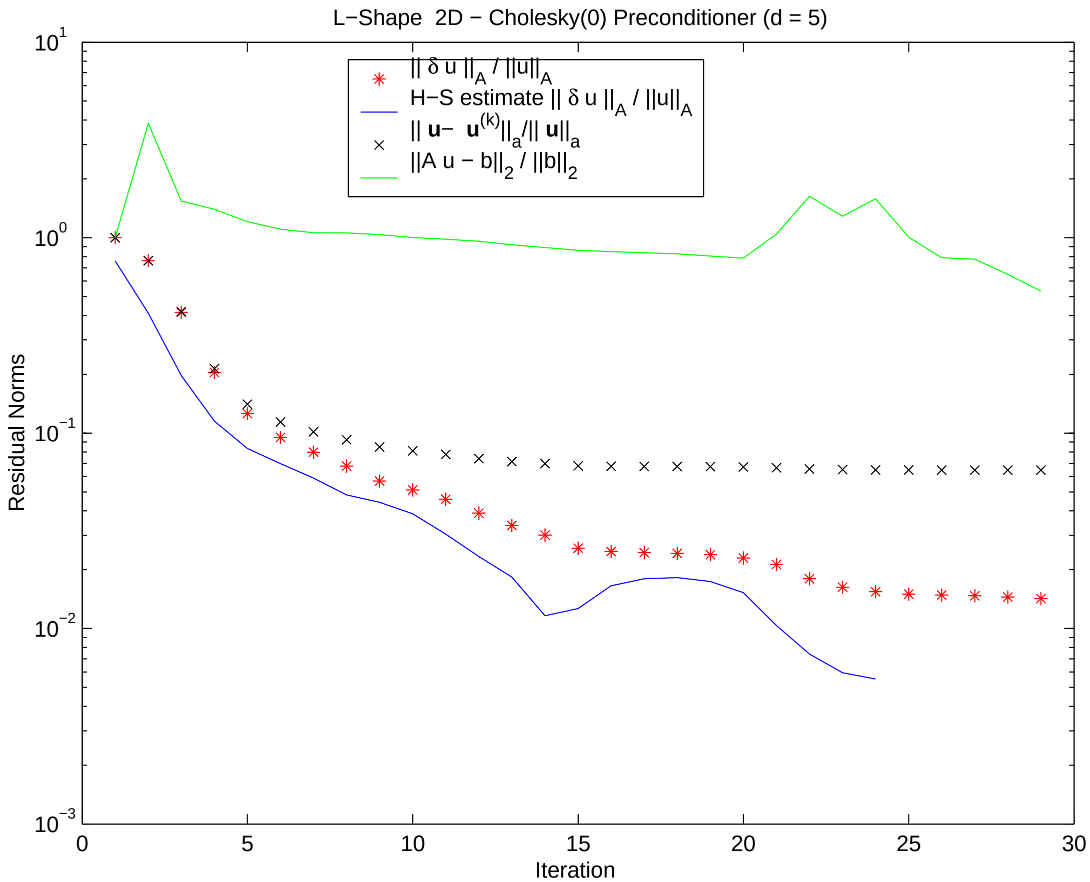
The condition numbers of the preconditioned matrices $\mathbf{M}^{-1}\mathbf{A}$ for the second problem are are still very high, and only the incomplete Cholesky preconditioner with drop tolerance 10^{-2} is an effective choice.

Example: Problem 1



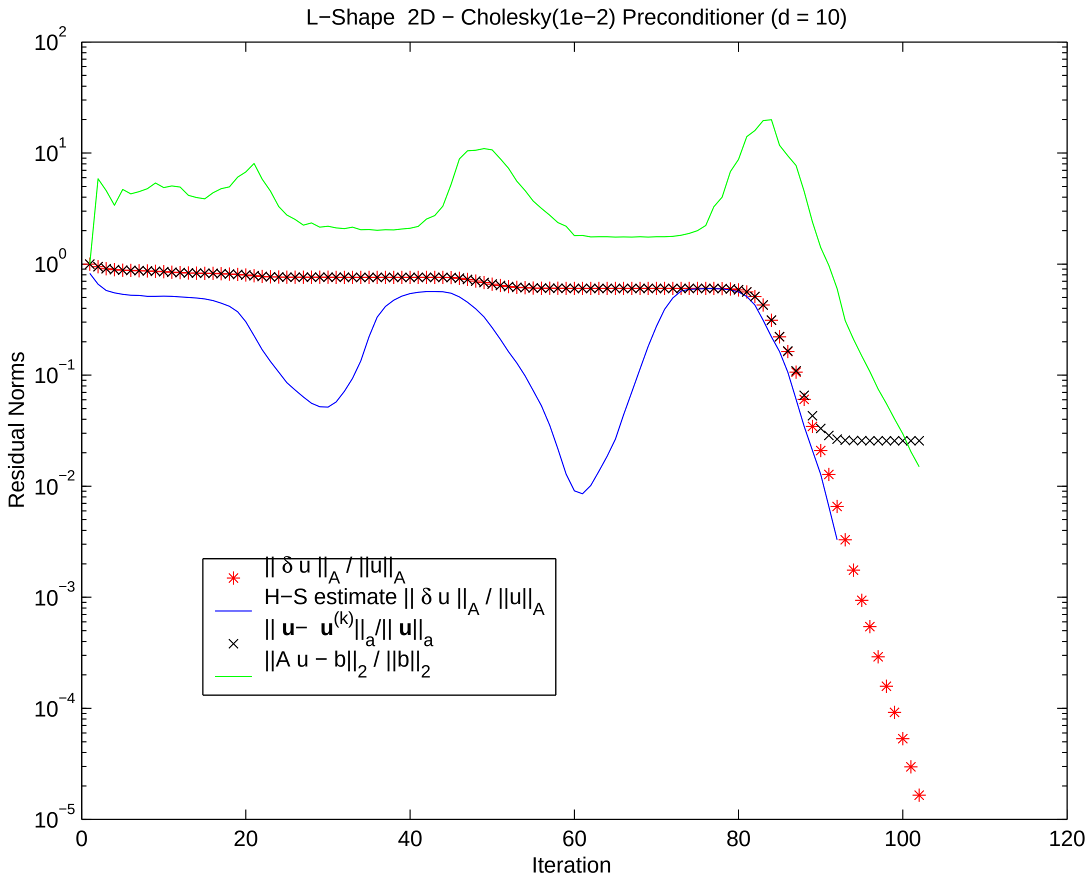
Behaviour of the norms of the residual for the Jacobi preconditioner.

Example: Problem 1



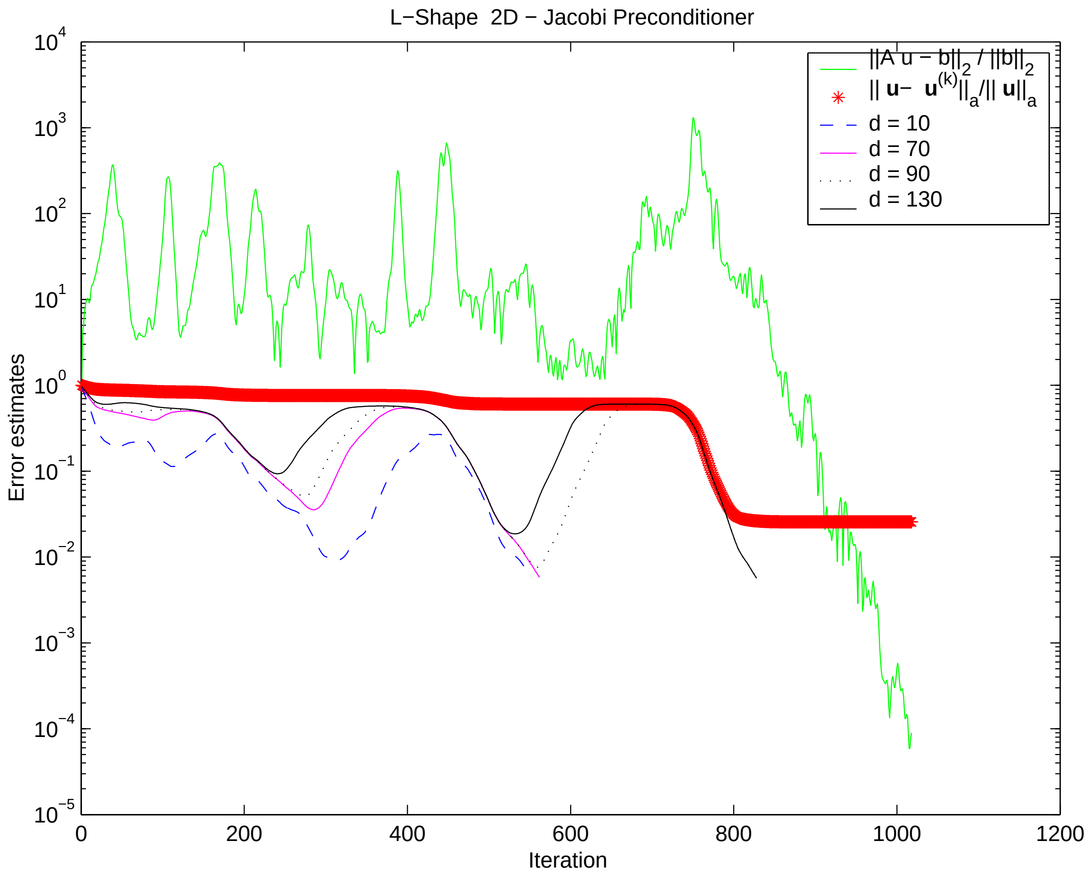
Behaviour of the norms of the residual for the incomplete Cholesky preconditioner.

Example: Problem 2



Behaviour of the norms of the residual for the incomplete Cholesky preconditioner with drop tolerance 10^{-2} and $d = 10$.

Example: Problem 2



Comparison of several estimates of the energy error for $d = 10, 70, 90, 130$ in Problem 2.

The positive definite problem

- $a(u,v) \neq a(v,u)$
- $\mathbf{A}$ asymmetric but positive definite
- $\mathbf{H} = \frac{1}{2}(\mathbf{A}^T + \mathbf{A})$ SPD

How to calculate $\|\mathbf{r}^{(k)}\|_{\mathbf{H}^{-1}}$?

- Solve preconditioned system

$$\mathbf{H}^{-1/2}\mathbf{A}\mathbf{H}^{-1/2}\hat{\mathbf{u}} = \mathbf{H}^{-1/2}\mathbf{b}$$

  - $\|\hat{\mathbf{r}}^{(k)}\|_{l_2} = \|\mathbf{r}^{(k)}\|_{\mathbf{H}^{-1}}$
  - 3-term recurrence
- Approximate it from Krylov subspace information.

See A., Login, and Wathen RAL-TR-2003-009

Current reports available at www.numerical.rl.ac.uk/reports/reports.shtml

One crime

Replace

$$\|u - u_h\|_{\mathcal{H}_h} \leq C(h)$$

with

$$\|u - u_h^{(k)}\|_{\mathcal{H}_h} \leq C(h)$$

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Sufficient condition

$$\|u - u_h\|_{\mathcal{H}_h} + \|u_h - u_h^{(k)}\|_{\mathcal{H}_h} \sim O(C(h))$$

$$\Downarrow$$

$$\|u_h - u_h^{(k)}\|_{\mathcal{H}_h} \sim O(C(h))$$

Stopping criteria

A general stopping criterion:

$$\|u_h - u_h^{(k)}\|_{\mathcal{H}_h} = \|\mathbf{u} - \mathbf{u}^{(k)}\|_{\mathbf{H}} \le C(h)$$

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Residual equation

$$\mathbf{r}^{(k)} = \mathbf{A}(\mathbf{u} - \mathbf{u}^{(k)})$$

$$\Downarrow$$

$$\|\mathbf{u} - \mathbf{u}^{(k)}\|_{\mathbf{H}} = \|\mathbf{A}^{-1}\mathbf{r}^{(k)}\|_{\mathbf{H}} = \|\mathbf{r}^{(k)}\|_{\mathbf{A}^{-T}\mathbf{H}\mathbf{A}^{-1}} \leq C(h)$$

Stopping criteria

Lemma *Let (inf-sup) hold. Then*

$$\|\mathbf{r}^{(k)}\|_{\mathbf{A}^{-T}\mathbf{H}\mathbf{A}^{-1}} \leq C_2^{-1}\|\mathbf{r}^{(k)}\|_{\mathbf{H}^{-1}}.$$

Stopping criteria

Lemma *Let (inf-sup) hold. Then*

$$\|\mathbf{r}^{(k)}\|_{\mathbf{A}^{-T}\mathbf{H}\mathbf{A}^{-1}} \leq C_2^{-1}\|\mathbf{r}^{(k)}\|_{\mathbf{H}^{-1}}.$$

New stopping criterion

$$\|\mathbf{r}^{(k)}\|_{\mathbf{H}^{-1}} \leq C_2 C(h)\|\mathbf{u}^{(k)}\|_{\mathbf{H}}.$$

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Examples

Elliptic problems in $\mathbb{R}^2$ (Ω unit square)

$$\begin{aligned} -\nabla\cdot(\mathbf{a}(\mathbf{x})\nabla u) + \mathbf{b}(\mathbf{x})\cdot\nabla u + c(\mathbf{x})u &= f \qquad \text{in } \Omega \\ u &= 0 \qquad \text{on } \Gamma. \end{aligned}$$

where

$$(\mathbf{a})_{ij},\ (\mathbf{b})_i,\ c \in \mathbf{L}^\infty(\Omega), \quad i,j = 1,2,$$

$$k_2(\mathbf{x})\,|\boldsymbol{\xi}|^2 \le \boldsymbol{\xi}^t\mathbf{a}(\mathbf{x})\boldsymbol{\xi} \le k_1(\mathbf{x})\,|\boldsymbol{\xi}|^2\,,$$

$$c(\mathbf{x}) - \frac{1}{2}\nabla\cdot\mathbf{b}(\mathbf{x}) \ge 0 \quad \forall\mathbf{x}\in\Omega.$$

Examples

$$a(w,v) = (\mathbf{a} \cdot \nabla w, \nabla v) + (\mathbf{b} \cdot \nabla w, v) + (cw, v),$$

is continuous and coercive with

$$C_1 = \|k_1\|_{L^\infty(\Omega)} + \|\mathbf{b}\|_{L^\infty(\Omega)} + C(\Omega)\|c\|_{L^\infty(\Omega)},$$

$$C_2 = \min_{\mathbf{x}\in\Omega} k_2(\mathbf{x}),$$

wrt $\|\cdot\|_{\mathcal{H}} = |\cdot|_{H_0^1(\Omega)} := |\cdot|_1$.

Examples

Error estimate:

$$|u - u_h|_1 \le C h^{s-1} \|u\|_s, \qquad 1 \le s \le 2.$$

Examples

Error estimate:

$$|u - u_h|_1 \leq Ch^{s-1}\|u\|_s, \qquad 1 \leq s \leq 2.$$

Issues

- What is h?
- How to approximate $\|u\|_s$?

Numerical experiments

- Discretization:
  linear elements on uniform & adaptive meshes

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- Discretization:
  linear elements on uniform & adaptive meshes
- Estimation of parameters

$$h \sim \frac{\|\mathbf{u}^k\|_{\mathbf{M}}}{\|\mathbf{u}^k\|_{l_2}}, \quad \|u\|_s \sim \|\mathbf{A}\mathbf{u}^k\|_{l_2}$$

Numerical experiments

Stopping criteria and estimates

- Residual dual norm: $\|\mathbf{r}^k\|_{\mathbf{H}^{-1}}$

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Stopping criteria and estimates

- Residual dual norm: $\|\mathbf{r}^k\|_{\mathbf{H}^{-1}}$
- Energy estimate $\|\mathbf{u}^k - \mathbf{u}^{k-1}\|_H \leq C_2 h^2 \|\mathbf{A}\mathbf{u}^k\|_{l_2}$

Advection-diffusion problem

$$\begin{aligned} -\varepsilon \Delta u + \mathbf{b} \cdot \nabla u &= f \qquad \text{in } \Omega \\ u &= g \qquad \text{on } \Gamma. \end{aligned}$$

$$\mathbf{b} = (2y(1-x^2), -2x(1-y^2)),$$

$$u(x,y) = x \left(\frac{1 - e^{\frac{y-1}{\varepsilon}}}{1 - e^{-\frac{2}{\varepsilon}}} \right),$$

$$\|v_h\|^2_{\mathcal{H}_h} = \varepsilon |v_h|_1^2 + \sum_{T \in \mathcal{T}^h} \delta_T \|\mathbf{b} \cdot \nabla v_h\|^2_{0,T}$$

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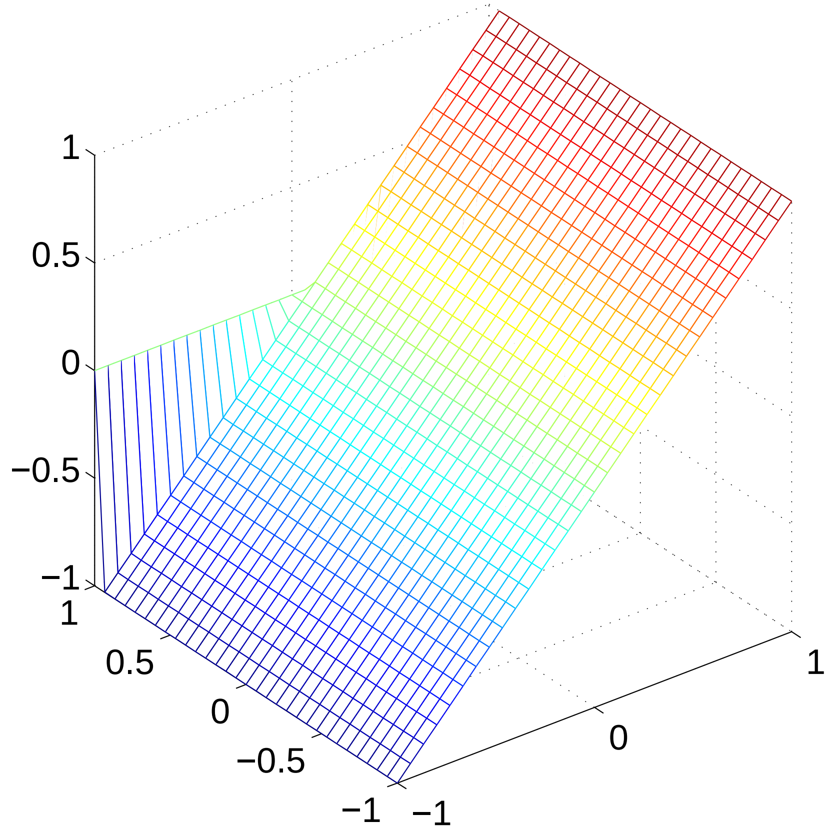
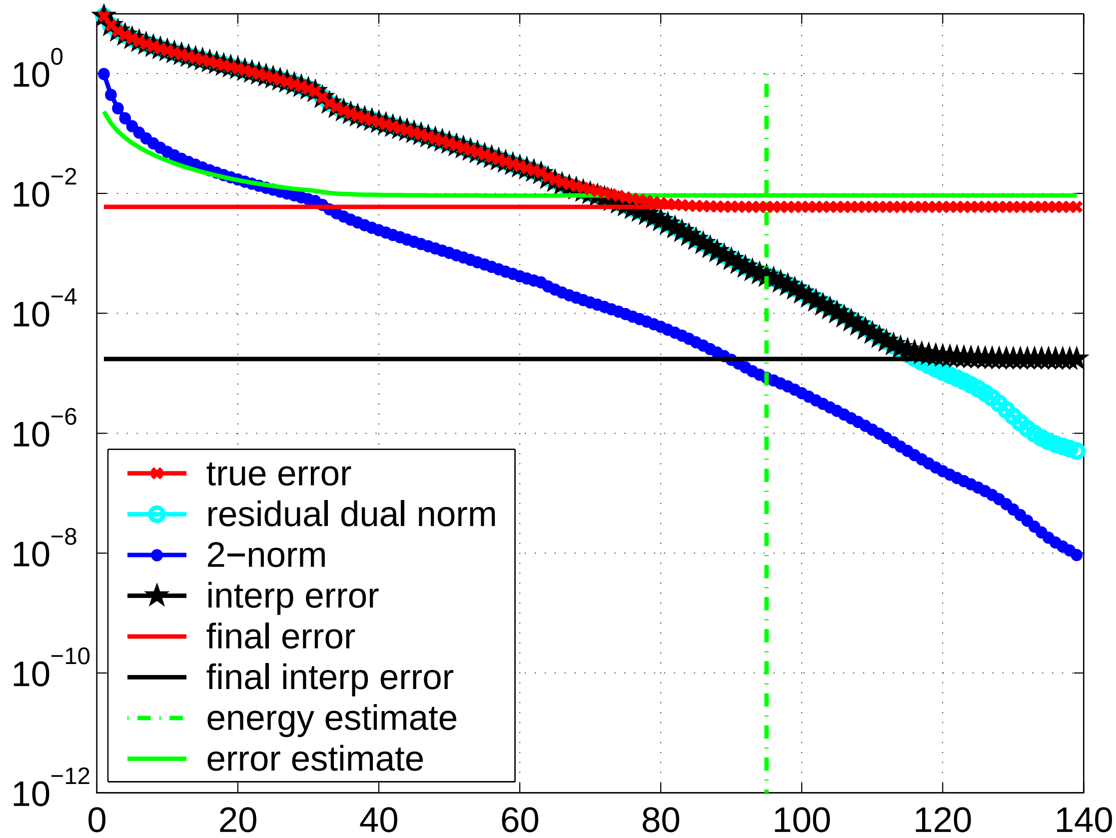
Advection-diffusion problem



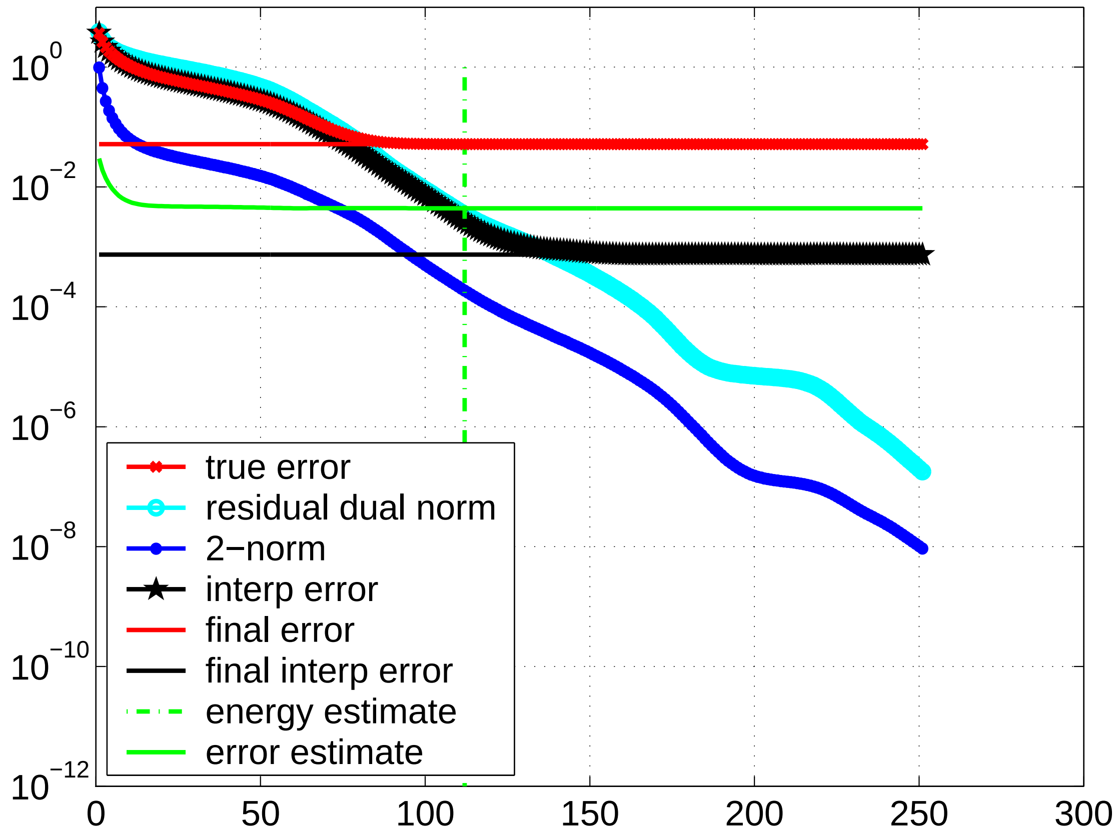
$$\varepsilon = 10^{-2}$$

Advection-diffusion problem



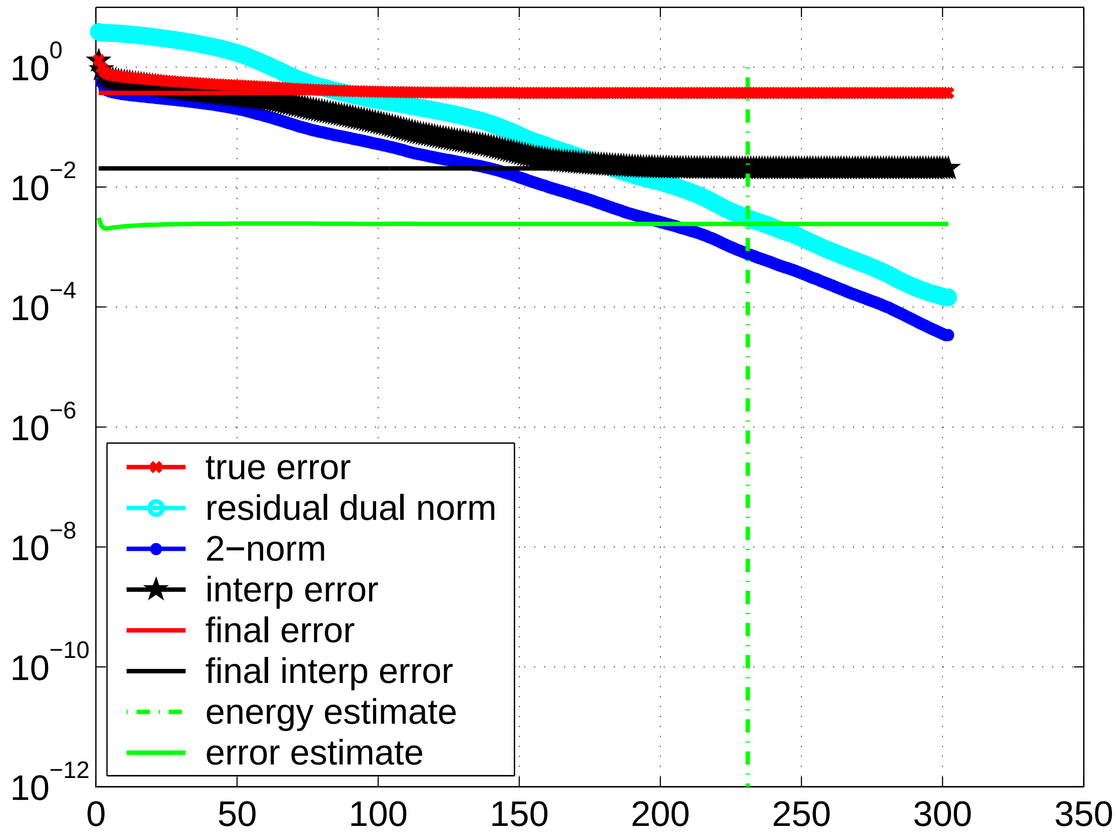
Uniform mesh; $\varepsilon = 1$

Advection-diffusion problem



Uniform mesh; $\varepsilon = 10^{-1}$

Advection-diffusion problem



Uniform mesh; $\varepsilon = 10^{-2}$

How to calculate $\|\mathbf{r}^k\|_{\mathbf{H}^{-1}}$?

- Solve preconditioned system

$$\mathbf{H}^{-1/2}\mathbf{A}\mathbf{H}^{-1/2}\hat{\mathbf{u}} = \mathbf{H}^{-1/2}\mathbf{f}$$

  - $\|\hat{\mathbf{r}}^k\|_{l_2} = \|\mathbf{r}^k\|_{H^{-1}}$
  - 3-term recurrence.

- Approximate it from Krylov subspace information.

How to calculate $\|\mathbf{r}^k\|_{H^{-1}}$?

- Concus & Golub, Widlund: 3-term recurrences for nonsymmetric problems
  - work in $\mathbf{H}$-inner product
  - do not minimize the residual norm.

Recall

$$\mathcal{K}_k(\mathbf{r}^0, \mathbf{A}) = \text{span}\left\{\mathbf{r}^0, \mathbf{A}\mathbf{r}^0, \ldots, \mathbf{A}^{k-1}\mathbf{r}^0\right\}$$

Arnoldi process

$$\mathbf{V}_k^T \mathbf{A} \mathbf{V}_k = \mathbf{H}_k$$

where $\mathbf{V}_k^T \mathbf{V}_k = I_k$ and $\mathbf{H}_k$= Hessenberg.

How to calculate $\|\mathbf{r}^k\|_{H^{-1}}$?

Lemma *Arnoldi applied to*

$$\mathcal{K}_k(\hat{\mathbf{r}}^0, \hat{\mathbf{A}}) \equiv \mathcal{K}_k(\mathbf{H}^{-1/2}\mathbf{r}^0, \mathbf{H}^{-1/2}\mathbf{A}\mathbf{H}^{-1/2})$$

and Arnoldi in the $\mathbf{H}$*-inner product applied to*

$$\mathcal{K}_k(\tilde{\mathbf{r}}^0, \tilde{A}) \equiv \mathcal{K}_k(\mathbf{H}^{-1}\mathbf{r}^0, \mathbf{H}^{-1}\mathbf{A})$$

produce the same $\mathbf{H}_k$. Moreover,

$$(\mathbf{H}_k)_{ij} = 0, \qquad |i - j| > 1.$$

Conclusions and future work

- The natural norm for FEM problems is the residual dual norm;
- Estimation is possible;
- For non-symmetric problems, preconditioning with the norm is useful;
- Reliable estimates for finite element error are required;
- Application to indefinite/saddle-point problems.

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FINAL MESSAGE: DO NOT ACCURATELY COMPUTE THE SOLUTION OF AN INACCURATE PROBLEM