



Matrix square root and interpolation spaces

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Outline

- Norms and duality in finite dimensional Hilbert spaces
- Discrete Interpolation Norms
- The continuous case and finite-element approximation
- An example: the biharmonic operator
- Summary and open problems



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Identify the norms for which we have

$$c ||v||_1 \leq ||v||_2 \leq C ||v||_1$$



Finite dimensional Hilbert spaces and \mathbf{R}^N

- $(\cdot, \cdot) : \mathcal{H} \times \mathcal{H} \rightarrow \mathbf{R}$ **scalar product** and
 $\|u\|_{\mathcal{H}} = \sqrt{(u, u)} \quad \forall u \in \mathcal{H}$ **norm**.



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■ $\exists \{\psi_i\}_{i=1, \dots, N}$ a basis for \mathcal{H}

$$\forall u \in \mathcal{H} \quad u = \sum_{i=1}^N u_i \psi_i \quad u_i \in \mathbf{R} \quad i = 1, \dots, N$$



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■ **Representation of scalar product in \mathbf{R}^N .**

$$\text{Let } u = \sum_{i=1}^N u_i \psi_i \text{ and } v = \sum_{i=1}^N v_i \psi_i.$$

Then

$$(u, v) = \sum_{i=1}^N \sum_{j=1}^N u_i v_j (\psi_i, \psi_j) = \mathbf{v}^T \mathbf{H} \mathbf{u}$$

where $\mathbf{H}_{ij} = \mathbf{H}_{ji} = (\psi_i, \psi_j)$ and $\mathbf{u}, \mathbf{v} \in \mathbf{R}^N$.

Moreover, $\mathbf{u}^T \mathbf{H} \mathbf{u} > 0$ iff $\mathbf{u} \neq 0$ and, thus \mathbf{H} **SPD**.



Dual space \mathcal{H}'

- $f \in \mathcal{H}' : \mathcal{H} \rightarrow \mathbf{R}$ (**functional**);
- $f(\alpha u + \beta v) = \alpha f(u) + \beta f(v) \quad \forall u, v \in \mathcal{H}$
- \mathcal{H}' is the space of the linear functionals on \mathcal{H}

$$\|f\|_{\mathcal{H}'} = \sup_{u \neq 0} \frac{f(u)}{\|u\|_{\mathcal{H}}}$$



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- **Dual vector**

Let $u \in \mathcal{H}$, $u \neq 0$, then $\exists f_u \in \mathcal{H}'$ such that

$$f_u(u) = \|u\|_{\mathcal{H}}$$

(Hahn-Banach).



Dual space \mathcal{H}'

- Let \mathcal{H} be a Hilbert finite dimensional space and \mathbf{H} the real $\mathbf{N} \times \mathbf{N}$ matrix identifying the scalar product.



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$$\mathbf{f} = \frac{\mathbf{H} \mathbf{u}}{\|\mathbf{u}\|_{\mathbf{H}}}$$

and

$$\|f_u\|_{\mathcal{H}'}^2 = \mathbf{u}^T \mathbf{H} \mathbf{u} = \mathbf{f}^T \mathbf{H}^{-1} \mathbf{f}$$



Linear operator

■ $A : \mathcal{H} \rightarrow \mathcal{V}$ and \mathcal{V} finite dimensional Hilbert spaces.



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$$\|\mathbf{A}\|_{\mathcal{H},\mathcal{V}} = \max_{\mathbf{u} \neq 0} \frac{\|\mathbf{A}\mathbf{u}\|_{\mathcal{V}}}{\|\mathbf{u}\|_{\mathcal{H}}} = \|\mathbf{V}^{1/2} \mathbf{A} \mathbf{H}^{-1/2}\|_2$$



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■ The result follows from the generalized eigenvalue problem in \mathbf{R}^N

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$$\kappa_H(M) = \|M\|_{H,H^{-1}} \|M^{-1}\|_{H^{-1},H}.$$



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$$\kappa_H(M) = \|M\|_{H,H^{-1}} \|M^{-1}\|_{H^{-1},H}.$$

The interesting case is $\kappa_H(M)$ independent of N



Interpolation spaces

$$\begin{aligned}\mathcal{H} &= (\mathbf{R}^N, (\mathbf{u}, \mathbf{v})_{\mathcal{H}} = \mathbf{u}^T H \mathbf{v}) \\ \mathcal{M} &= (\mathbf{R}^N, (\mathbf{u}, \mathbf{v})_{\mathcal{M}} = \mathbf{u}^T M \mathbf{v})\end{aligned}$$

$$(\mathbf{u}, \mathbf{v})_{\mathcal{H}} = (\mathbf{u}, \mathbf{S}\mathbf{v})_{\mathcal{M}} = (\mathbf{S}\mathbf{u}, \mathbf{v})_{\mathcal{M}}$$

$$\mathbf{S} = M^{-1}H$$

S self-adjoint in the good scalar product!

$$\left\{ \mathbf{S}\mathbf{x} = \mu\mathbf{x} \quad \Leftrightarrow \quad H\mathbf{x} = \mu M\mathbf{x} \right\} \Rightarrow \mu = \delta^2 > 0$$

$$\exists W \text{ s.t. } M = W^T W, \quad H = W^T \Delta^2 W, \quad \Delta \text{ diagonal}$$



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Interpolation spaces

$$\mathbf{\Lambda} = W^{-1}\Delta W \quad \mathbf{\Lambda}^{1/2} = W^{-1}\Delta^{1/2}W$$

$$\begin{aligned} \mathbf{S} = M^{-1}H &= W^{-1}W^{-T}W^T\Delta^2W \\ &= W^{-1}\Delta WW^{-1}\Delta W \\ &= \mathbf{\Lambda}^2 \end{aligned}$$

$$M\mathbf{\Lambda} = W^TWW^{-1}\Delta W^{-T}W^TW = \mathbf{\Lambda}^T M \Rightarrow (\mathbf{u}, \mathbf{\Lambda}\mathbf{v})_{\mathcal{M}} = (\mathbf{\Lambda}\mathbf{u}, \mathbf{v})_{\mathcal{M}}$$

$$(\mathbf{\Lambda}^{1/2}\mathbf{u}, \mathbf{\Lambda}^{1/2}\mathbf{u})_{\mathcal{M}} = (\mathbf{u}, \mathbf{\Lambda}\mathbf{u})_{\mathcal{M}}$$



Interpolation spaces

$$[\mathcal{H}, \mathcal{M}]_{\vartheta} = \left\{ \mathbf{u} \in \mathbf{R}^N; \left((\mathbf{u}, \mathbf{u})_{\mathcal{M}} + (\mathbf{u}, S^{1-\vartheta} \mathbf{u})_{\mathcal{M}} \right)^{1/2} \right\}$$

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$$\|v\|_{\vartheta}^2 = \|v\|_{H_{\vartheta}}^2 = v^T \left(M + MS^{1-\vartheta} \right) v$$

$$H_{\vartheta} = M \left(I + S^{1-\vartheta} \right) = W^T \left(I + \Delta^{2(1-\vartheta)} \right) W$$



Interpolation spaces (duality)

\mathcal{M}' and \mathcal{H}' dual spaces of \mathcal{M} and \mathcal{H}

$$\left[\mathcal{H}, \mathcal{M} \right]_{\vartheta}' = \left[\mathcal{M}', \mathcal{H}' \right]_{1-\vartheta}$$

$$S' = MH^{-1} = W^T \Delta^{-2} W^{-T}$$



Interpolation spaces (duality)

\mathcal{M}' and \mathcal{H}' dual spaces of \mathcal{M} and \mathcal{H}

$$\left[\mathcal{H}, \mathcal{M} \right]_{\vartheta}' = \left[\mathcal{M}', \mathcal{H}' \right]_{1-\vartheta}$$

$$S' = M H^{-1} = W^T \Delta^{-2} W^{-T}$$

$$H'_{1-\vartheta} = H_{1-\vartheta}^{-1} = W^{-1} \Delta^{-2\vartheta} W^{-T}$$



Interpolation spaces (∞ dimension case)

- X, Y two Hilbert spaces with $X \subset Y$, X dense and continuously embedded in Y . $\langle \cdot, \cdot \rangle_X, \langle \cdot, \cdot \rangle_Y$ and $\| \cdot \|_X, \| \cdot \|_Y$ the respective norms.
- (Riesz representation theory) $\exists \mathcal{J} : X \rightarrow Y$ positive and self-adjoint with respect to $\langle \cdot, \cdot \rangle_Y$ such that $\langle u, v \rangle_X = \langle u, \mathcal{J}v \rangle_Y$.
 $\mathcal{E} = \mathcal{J}^{1/2} : X \rightarrow Y,$
- $X = D(\mathcal{E})$ with $\|u\|_X \sim \|u\|_{\mathcal{E}} := (\|u\|_Y^2 + \|\mathcal{E}u\|_Y^2)^{1/2}$.
- $\|u\|_{\theta} := (\|u\|_Y^2 + \|\mathcal{E}^{1-\theta}u\|_Y^2)^{1/2}$.
- The *interpolation space of index θ* $[X, Y]_{\theta} := D(\mathcal{E}^{1-\theta}), 0 \leq \theta \leq 1,$ with the inner-product $\langle u, v \rangle_{\theta} = \langle u, v \rangle_Y + \langle u, \mathcal{E}^{1-\theta}v \rangle_Y$ is a Hilbert space (Lions Magenes 1968).
- $[X, Y]_0 = X$ and $[X, Y]_1 = Y$. If $0 < \theta_1 < \theta_2 < 1$ then
$$X \subset [X, Y]_{\theta_1} \subset [X, Y]_{\theta_2} \subset Y.$$
- $\forall \theta \in (0, 1) \pi \in \mathcal{L}(X; \mathcal{X}) \cap \mathcal{L}(Y; \mathcal{Y}) \implies \pi \in \mathcal{L}([X, Y]_{\theta}; [\mathcal{X}, \mathcal{Y}]_{\theta}).$



Interpolation spaces (∞ dimension case)

$\Omega \subset \mathbb{R}^n$ open bounded with smooth boundary Γ and let α denote a multi-index of order m where m is a positive integer

$$H^m(\Omega) = \{u : D^\alpha u \in L^2(\Omega), \quad |\alpha| \leq m\} \quad (H^0(\Omega) = L^2(\Omega))$$

$$H^s(\Omega) := [H^m(\Omega), H^0(\Omega)]_{1-s/m}$$

$H_0^s(\Omega)$ completion of $C_0^\infty(\Omega)$ in $H^m(\Omega)$, where $s > 0$. For $0 \leq s_2 < s_1$,

$$\begin{cases} [H_0^{s_1}(\Omega), H_0^{s_2}(\Omega)]_\theta = H_0^{(1-\theta)s_1 + \theta s_2}(\Omega) & \text{if } (1-\theta)s_1 + \theta s_2 \neq k + 1/2 \\ [H_0^{s_1}(\Omega), H_0^{s_2}(\Omega)]_\theta = H_{00}^{k+1/2}(\Omega) \subset H_0^{k+1/2}(\Omega) & \text{if } (1-\theta)s_1 + \theta s_2 = k + 1/2 \end{cases}$$

$$H^{-s}(\Omega) = (H_0^s(\Omega))' \quad s > 0$$

If $(1-\theta)s_1 + \theta s_2 = 1/2$

$$[H^{-s_1}(\Omega), H^{-s_2}(\Omega)]_\theta = \left(H_{00}^{1/2}(\Omega) \right)'$$



Finite-element example

$$H_{00}^{1/2}(\Omega) = [H_0^1(\Omega), L^2(\Omega)]_{1/2}.$$

Let $X_h \subset H_0^1(\Omega)$, $Y_h \subset L^2(\Omega)$. Let $\{\phi_i\}_{1 \leq i \leq n} \in X_h$ be a spanning set for Y_h and let $L_k \in \mathbb{R}^{n \times n}$ denote the Grammian matrices corresponding to the $\langle \cdot, \cdot \rangle_{H_0^k(\Omega)}$ -inner product ($H^0(\Omega) = L^2(\Omega)$):

$$(L_k)_{ij} = \langle \phi_i, \phi_j \rangle_{H_0^k(\Omega)}.$$

$H = L_1$, $M = L_0$ and

$$H_{1/2,h} = L_0 \left(I + (L_0^{-1} L_1)^{1/2} \right)$$

Moreover, we have

$$H_{1/2,h} \sim H_{1/2} = L_0 \left(L_0^{-1} L_1 \right)^{1/2}$$



Finite-element example

$$\left(H_{00}^{1/2}(\Omega)\right)' = [H^{-(1)}(\Omega), H^0(\Omega)]_{1/2} = ([H_0^1(\Omega), H_0^0(\Omega)]_{1/2})'.$$

Let X_h, Y_h be defined as above. Let $Y_h' \subset X_h' = \text{span} \{\psi_i\}_{1 \leq i \leq n}$ where ψ_i are basis functions dual to ϕ_i , i.e., $\langle \psi_i, \phi_j \rangle_{H^{-1}(\Omega) \times H_0^1(\Omega)} = \delta_{ij}$.

$$\text{If } Y_h' \ni z = \sum_{i=1}^n \mathbf{z}_i \psi_i = \sum_{i=1}^n \mathbf{w}_i \phi_i, \quad \phi_l = \sum_{i=1}^n K_{li} \psi_i$$

$$\delta_{ij} = \langle \psi_i, \phi_j \rangle_{H^{-1}(\Omega) \times H_0^1(\Omega)} = \sum_{l=1}^n K_{il}^{-1} \langle \phi_l, \phi_j \rangle_{H_0^1(\Omega)} = \sum_{l=1}^n K_{il}^{-1} (L_1)_{lj}$$

so that $\mathbf{z} = L_0 \mathbf{w}$ and $\|\mathbf{z}\|_{H_Y'} = \|\mathbf{w}\|_{L_0^{-1}}$, $\|\mathbf{z}\|_{H_X'} = \|\mathbf{w}\|_{L_0 L_1^{-1} L_0}$ and the matrix representation of H_Y', H_X' are respectively L_0 and $L_0 L_1^{-1} L_0$.

$$H_{1/2}' = L_0 (L_0^{-1} L_1)^{-1/2} = H_{-1/2}.$$



Evaluation of $H_{\theta z}$

■ Generalised Lanczos

$$H_X V_k = H_Y V_k T_k + \beta_{k+1} H_y \mathbf{v}_{k+1} \mathbf{e}_k^T, \quad V_k^T H_Y V_k = I_k$$

(T_k tridiagonal).



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■ $\mathbf{v}_0 = \mathbf{z}$

$$H_\theta \mathbf{z} \approx H_Y V_k T_k^{1-\theta} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y} \text{ and}$$

$$H_{\theta,h} \mathbf{z} \approx H_Y V_k (I_k + T_k^{1-\theta}) \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}.$$



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■ Alternative: N. Hale, and N. J. Higham and L. N. Trefethen, *SIAM J. Numer. Anal.*



An example: biharmonic operator

Consider the biharmonic problem in a polygonal convex open domain $\Omega \subset \mathbb{R}^2$ with boundary $\Gamma = \cup_{i=1}^K \Gamma_i$.

$$\begin{cases} \Delta^2 u = f & \text{in } \Omega, \\ u = \partial u / \partial n = 0 & \text{on } \Gamma. \end{cases}$$

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ v + \Delta u = 0 & \text{in } \Omega, \\ u = \partial u / \partial n = 0 & \text{on } \Gamma. \end{cases}$$



An example: biharmonic operator

(Pironneau-Glowinski)

$$\begin{aligned} \text{(i)} \quad & \left\{ \begin{array}{ll} -\Delta v_0 = f & \text{in } \Omega, \\ v_0 = 0 & \text{on } \Gamma, \end{array} \right. & \left\{ \begin{array}{ll} -\Delta u_0 = v_0 & \text{in } \Omega, \\ u_0 = 0 & \text{on } \Gamma, \end{array} \right. \\ \text{(ii)} \quad & \mathcal{S}\lambda = \partial u_0 / \partial \nu \quad \text{on } \Gamma, \\ \text{(iii)} \quad & \left\{ \begin{array}{ll} -\Delta v_1 = 0 & \text{in } \Omega, \\ v_1 = \lambda & \text{on } \Gamma, \end{array} \right. & \left\{ \begin{array}{ll} -\Delta u_1 = v_1 & \text{in } \Omega, \\ u_1 = 0 & \text{on } \Gamma, \end{array} \right. \end{aligned}$$



An example: biharmonic operator

\mathcal{S} is a boundary operator which is defined on $H^{-1/2}(\Gamma)$ and which induces a bilinear form

$$s(\cdot, \cdot) : H^{-1/2}(\Gamma) \times H^{-1/2}(\Gamma)$$

$s(\cdot, \cdot)$ is symmetric, positive-definite and $H^{-1/2}(\Gamma)$ -elliptic, i.e.,

$$c_1 \|\lambda\|_{H^{-1/2}(\Gamma)}^2 \leq s(\lambda, \lambda) \leq c_2 \|\lambda\|_{H^{-1/2}(\Gamma)}^2.$$



An example: biharmonic operator

$$\begin{pmatrix} L & Z \\ Z^T & -M_{BB} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{v}_B \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ 0 \end{pmatrix}$$

The Schur complement associated with L in the matrix is

$$S = -M_{BB} - Z^T L^{-1} Z.$$

Let $X_h \subset H^1(\Gamma)$ denote the space spanned by the restriction of the basis functions of V_I^h to the boundary Γ . If $\lambda_h \in X_h$ has a vector of coefficients $\boldsymbol{\lambda}$, then

$$s(\lambda_h, \lambda_h) = \boldsymbol{\lambda}^T S \boldsymbol{\lambda}.$$



An example: biharmonic operator

A discrete $H^{-1/2}$ -norm on X_h can be defined as a sum of norms corresponding to each *open* segment of the polygonal boundary Γ :

$$\|\lambda_h\|_{H^{-1/2}(\Gamma)} := \left(\sum_{i=1}^K \|\lambda_h\|_{H^{-1/2}(\Gamma_i)}^2 \right)^{1/2}.$$

In particular, $H^{-1/2}(\Gamma_i) = (H_{00}^{1/2}(\Gamma_i))'$.

$$\|\lambda_h\|_{H^{-1/2}(\Gamma)}^2 = \|\boldsymbol{\lambda}\|_{H_{\{-1/2,h\}}}^2 \quad \left(\text{or} \quad = \|\boldsymbol{\lambda}\|_{H_{\{-1/2\}}}^2 \right)$$

for $\lambda_h \in X_h$ where

$$H_{\{-1/2,h\}} = \bigoplus_{i=1}^K H_{1/2,h}^{\{i\}}$$

$$\left(H_{\{-1/2\}} = \bigoplus_{i=1}^K H_{-1/2}^{\{i\}}, \quad H_{-1/2}^{\{i\}} = L_{0,i} (L_{0,i}^{-1} L_{1,i})^{-1/2} \right)$$



An example: biharmonic operator

$$P = \begin{pmatrix} L & Z \\ & P_S \end{pmatrix}$$



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n	m	I	$H_{\{-1/2, h\}}$	$H_{\{-1/2\}}$	$\hat{H}_{\{-1/2\}}$
84,610	640	26	10	12	12
337,154	1,280	30	9	11	11
1,346,050	2,560	36	9	11	11

FGMRES iterations for model problem .



Open problems

- Domain decomposition: preliminary results show total independence from mesh size



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- Domain decomposition: preliminary results show total independence from mesh size
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- 3D PDEs



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- For which class of matrices the Schur complement is spectrally equivalent to an algebraic interpolation space matrix