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: Domain Decomposition
- Summary and open problems

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Identify the norms for which we have

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

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

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- Representation of scalar product in $\mathbf{R}^{\mathbb{N}}$.
  Let $u = \sum_{i=1}^{\mathbb{N}} u_i \psi_i$ and $v = \sum_{i=1}^{\mathbb{N}} v_i \psi_i$.
  Then

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

  where $\mathbf{H}_{ij} = \mathbf{H}_{ji} = (\psi_i, \psi_j)$ and $\mathbf{u}, \mathbf{v} \in \mathbf{R}^{\mathbb{N}}$.
  Moreover, $\mathbf{u}^T \mathbf{H} \mathbf{u} > 0 \qquad$ iff $\qquad \mathbf{u} \neq 0$ and, thus $\mathbf{H}$ SPD.

Dual space $\mathcal{H}'$

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

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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).

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

  and

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

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

Interpolation spaces

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

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

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

$\mathbf{S}$ self-adjoint in the good scalar product!

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

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

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

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

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

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

Interpolation spaces

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

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

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

Interpolation spaces (duality)

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

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

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) $\exists \mathcal{J} : X \to Y$ positive and self-adjoint with respect to $\langle \cdot, \cdot \rangle_Y$ such that $\langle u, v \rangle_X = \langle u, \mathcal{J} v \rangle_Y$.
  $\mathcal{E} = \mathcal{J}^{1/2} : X \to Y$,
- $X = D(\mathcal{E})$ with $\|u\|_X \sim \|u\|_{\mathcal{E}} := \left(\|u\|_Y^2 + \|\mathcal{E} u\|_Y^2 \right)^{1/2}$.
- $\|u\|_\theta := \left(\|u\|_Y^2 + \|\mathcal{E}^{1-\theta} u\|_Y^2 \right)^{1/2}$.
- The *interpolation space of index* θ $[X, Y]_\theta := D(\mathcal{E}^{1-\theta}), \;\; 0 \leq \theta \leq 1$, with the inner-product $\langle u, v \rangle_\theta = \langle u, v \rangle_Y + \left\langle u, \mathcal{E}^{1-\theta} v \right\rangle_Y$ is a Hilbert space (Lions Magenes 1968).
- $[X, Y]_0 = X$ and $[X, Y]_1 = Y$. If $0 < \theta_1 < \theta_2 < 1$ then

$$X \subset [X, Y]_{\theta_1} \subset [X, Y]_{\theta_2} \subset Y.$$

Interpolation Theorem

Let X, Y Hilbert spaces $X \subset Y$ with X dense in Y, and with inclusion compact and continuous. Let $\mathcal{X}, \mathcal{Y}$ satisfy similar properties. Let $\pi \in \mathcal{L}(X; \mathcal{X}) \cap \mathcal{L}(Y; \mathcal{Y})$. Then for all $\theta \in (0, 1)$,

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Let $X \supset X_h$ and $Y \supset Y_h$ finite-dimensional spaces $i_h : \mathcal{L}(X_h; X) \cap \mathcal{L}(Y_h; Y)$ the continuous injection operator

$$i_h \in \mathcal{L}([X_h, Y_h]_\theta; [X, Y]_\theta).$$

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Assume now that there exists an interpolation operator $\exists I_h$ such that $I_h : \mathcal{L}(X; X_h) \cap \mathcal{L}(Y; Y_h)$ and $I_h u = u_h$ for all $u_h \in X_h$.

$$I_h \in \mathcal{L}([X, Y]_\theta; [X_h, Y_h]_\theta)$$

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Since $[X_h, Y_h]_\theta \subset [X, Y]_\theta$

$$\frac{1}{C_1} \|u_h\|_\theta \leq \|u_h\|_{\theta,h} \leq C_2 \|u_h\|_\theta.$$

Interpolation spaces (∞ dimension case)

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

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

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

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

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

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

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 $\{\phi_i\}_{1\le i\le n} \in X_h$ 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 $(H^0(\Omega) = L^2(\Omega))$:

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

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

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

Moreover, we have

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

Finite-element example

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

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

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

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

so that $\mathbf{z} = L_0\mathbf{w}$ and $\|\mathbf{z}\|_{H_Y'} = \|\mathbf{w}\|_{L_0^{-1}}, \quad \|\mathbf{z}\|_{H_X'} = \|\mathbf{w}\|_{L_0 L_1^{-1} L_0}$ 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 $H_\theta \mathbf{z}$

- Generalised Lanczos
  $H_X V_k = H_Y V_k T_k + \beta_{k+1} H_y \mathbf{v}_{k+1} \mathbf{e}_k^T, \quad V_k^T H_Y V_k = I_k$
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- $\mathbf{v}_0 = \mathbf{z}$
  $H_\theta \mathbf{z} \approx H_Y V_k T_k^{1-\theta} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}$ 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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- $\mathbf{v}_0 = H_Y^{-1} \mathbf{z}$
  $H_\theta^{-1} \mathbf{z} \approx V_k T_k^{\theta-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}$ and
  $H_{\theta,h}^{-1} \mathbf{z} \approx V_k (I_k + T_k^{1-\theta})^{-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}$.

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  (T_k tridiagonal).
- $\mathbf{v}_0 = \mathbf{z}$
  $H_\theta \mathbf{z} \approx H_Y V_k T_k^{1-\theta} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}$ and
  $H_{\theta,h} \mathbf{z} \approx H_Y V_k (I_k + T_k^{1-\theta}) \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}$.
- $\mathbf{v}_0 = H_Y^{-1} \mathbf{z}$
  $H_\theta^{-1} \mathbf{z} \approx V_k T_k^{\theta-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}$ and
  $H_{\theta,h}^{-1} \mathbf{z} \approx V_k (I_k + T_k^{1-\theta})^{-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}$.
- Alternative: N. Hale, and N. J. Higham and L. N. Trefethen, SIAM J. Numer. Anal.

Preconditioners for the Steklov-Poincaré operator

Let Ω be an open subset of $\mathbb{R}^d$ with boundary $\partial\Omega$ and consider the model problem

$$\begin{cases} -\Delta u &= f \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega. \end{cases}$$

Given a partition of Ω into two subdomains $\Omega \equiv \Omega_1 \cup \Omega_2$ with common boundary Γ this problem can be equivalently written as

$$\begin{cases} -\Delta u_1 &= f \qquad \text{in } \Omega_1, \\ u_1 &= 0 \qquad \text{on } \partial\Omega_1 \setminus \Gamma, \end{cases} \qquad \begin{cases} -\Delta u_2 &= f \qquad \text{in } \Omega_2, \\ u_2 &= 0 \qquad \text{on } \partial\Omega_2 \setminus \Gamma, \end{cases}$$

with the ‘interface conditions’

$$\begin{cases} u_1 &= u_2 \\ \dfrac{\partial u_1}{\partial n_1} &= -\dfrac{\partial u_2}{\partial n_2} \end{cases} \quad \text{on } \Gamma$$

Preconditioners for the Steklov-Poincaré operator

Given $\lambda_1, \lambda_2 \in H_{00}^{1/2}(\Gamma)$, ψ_1, ψ_2 denote the harmonic extensions of λ_1, λ_2 respectively into Ω_1, Ω_2, i.e., for $i = 1, 2$, ψ_i satisfy

$$\begin{cases} -\Delta\psi_i &= 0 & \text{in } \Omega_i, \\ \psi_i &= \lambda_i & \text{on } \Gamma, \\ \psi_i &= 0 & \text{on } \partial\Omega_i \setminus \Gamma. \end{cases}$$

The Steklov-Poincaré operator $\mathcal{S} : H_{00}^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$

$$\langle \mathcal{S}\lambda_1, \lambda_2 \rangle_{H^{1/2}(\Gamma)} = \langle \nabla\psi_1, \nabla\psi_2 \rangle_{L^2(\Omega)} =: s(\lambda_1, \lambda_2).$$

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

Preconditioners for the Steklov-Poincaré operator

$$\text{(i)} \quad \begin{cases} -\Delta u_i^{\{1\}} &= f \ \text{ in } \Omega_i, \\ u_i^{\{1\}} &= 0 \ \text{ on } \partial\Omega_i, \end{cases}$$

$$\text{(ii)} \quad \left\{ \mathcal{S}\lambda = -\frac{\partial u_1^{\{1\}}}{\partial n_1} - \frac{\partial u_2^{\{1\}}}{\partial n_2} \ \text{ on } \Gamma, \right.$$

$$\text{(iii)} \quad \begin{cases} -\Delta u_i^{\{2\}} &= 0 \ \text{ in } \Omega_i, \\ u_i^{\{2\}} &= \lambda \ \text{ on } \partial\Omega_i. \end{cases}$$

The resulting solution is

$$u|_{\Omega_i} = u_i^{\{1\}} + u_i^{\{2\}}.$$

An other problem

$$\begin{cases} -\nu\Delta u + \vec{b}\cdot\nabla u &= f \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega. \end{cases}$$

Discrete Formulation

$$V^h = V^{h,r} := \left\{ w \in C^0(\Omega) : w|_{\mathfrak{t}} \in P_k \ \ \forall \mathfrak{t} \in \mathfrak{T}_h \right\} \subset H^1(\Omega)$$

be a finite-dimensional space of piecewise polynomial functions defined on some subdivision $\mathfrak{T}_h$ of Ω into simplices $\mathfrak{t}$ of maximum diameter h. Let further $V_I^h, V_B^h \subset V^h$ satisfy $V_I^h \oplus V_B^H \equiv V^h$ where $V_I^h = \left\{ w \in V^h : w|_{\partial\Omega} = 0 \right\}$. Let $X_h \subset H_0^1(\Gamma)$ denote the space spanned by the restriction of the basis functions of V_I^h to the internal boundary Γ.

Discrete Formulation

$$
\begin{aligned}
&\text{(i)} \quad & A_{II,i}\mathbf{u}_i^{\{1\}} &= \mathbf{f}_{I,i}, \\
&\text{(ii)} \quad & S\mathbf{u}_B &= \mathbf{f}_B - A_{IB,1}^T\mathbf{u}_1^{\{1\}} - A_{IB,2}^T\mathbf{u}_2^{\{2\}}, \\
&\text{(iii)} \quad & A_{II,i}\mathbf{u}_i^{\{2\}} &= -A_{IB,1}^T\mathbf{u}_B - A_{IB,2}^T\mathbf{u}_B,
\end{aligned}
$$

where S is the Schur complement corresponding to the boundary nodes

$$S = S_1 + S_2, \quad S_i = A_{BB,i} - A_{IB,i}^T A_{II,i}^{-1} A_{IB,i}.$$

The resulting solution is $(\mathbf{u}_{I,1},\ \mathbf{u}_{I,2},\ \mathbf{u}_B)$ where

$$\mathbf{u}_{I,i} = \mathbf{u}_i^{\{1\}} + \mathbf{u}_i^{\{2\}}.$$

$H_{00}^{1/2}$-preconditioners

Let $X_h = \text{span}\{\phi_i, 1 \le i \le m\}$ *be defined as above and let* $(L_k)_{ij} = \langle \phi_i, \phi_j \rangle_{H_0^k(\Gamma)}$ *for* $k = 0, 1$. *Let*

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

Then for all $\boldsymbol{\lambda} \in \mathbb{R}^m \setminus \{\mathbf{0}\}$

$$\kappa_1 \le \frac{\boldsymbol{\lambda}^T S \boldsymbol{\lambda}}{\boldsymbol{\lambda}^T H_{1/2} \boldsymbol{\lambda}} \le \kappa_2$$

with κ_1, κ_2 *independent of* h.

Discrete DD

$$P = \begin{pmatrix} A_{II} & A_{IB} \\ 0 & P_S \end{pmatrix}$$

with $A_{II} = \nu L_{II} + N_{II}$ where L_{II} is the direct sum of Laplacians assembled on each subdomain and N_{II} is the direct sum of the convection operator $\vec{b} \cdot \nabla$ assembled also on each subdomain.

Numerical results: Poisson equatione

			Linear			Quadratic		
$\#dom$	n	m	$H_{1/2,h}$	$H_{1/2}$	$\widehat{H}_{1/2}$	$H_{1/2,h}$	$H_{1/2}$	$\widehat{H}_{1/2}$
4	45,377	449	10	9	9	11	11	11
	180,865	897	10	10	10	11	11	11
	722,177	1793	11	11	11	11	11	11
16	45,953	1149	13	12	12	13	13	13
	183,041	2301	13	13	13	13	13	13
	730,625	4605	13	13	13	13	13	13
64	66,049	3549	16	14	14	16	15	15
	263,169	7133	16	15	15	16	15	15
	1,050,625	14,301	17	16	15	17	15	15

FGMRES iterations for model problem .

An other problem

			Linear			Quadratic		
$\#dom$	n	m	$\nu = 1$	$\nu = 0.1$	$\nu = 0.01$	$\nu = 1$	$\nu = 0.1$	$\nu = 0.01$
4	45,377	449	10	12	21	12	13	20
	180,865	897	11	11	20	12	13	19
	722,177	1793	11	11	19	12	12	18
16	45,953	1149	12	17	37	13	17	35
	183,041	2301	13	17	35	13	16	32
	730,625	4605	12	15	32	12	15	30
64	66,049	3549	16	22	55	17	21	51
	263,169	7133	17	22	52	16	20	46
	1,050,625	14,301	15	19	47	16	19	43

FGMRES iterations for 2nd model problem

Exotic domains

- QUANTUM graphs (metric graph)

Exotic domains

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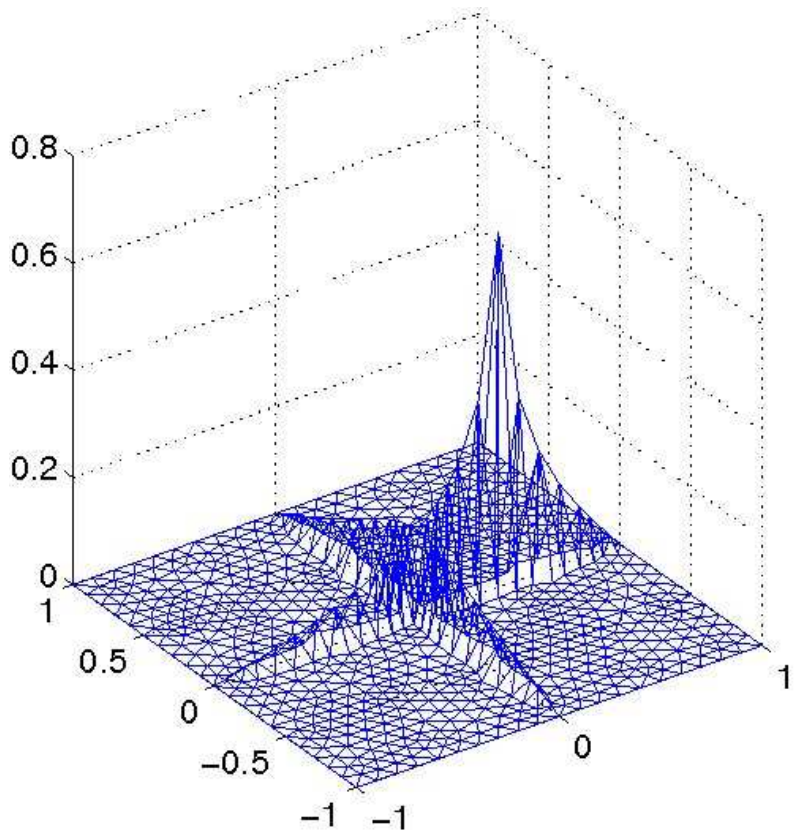
- 2-D simplex

Exotic domains

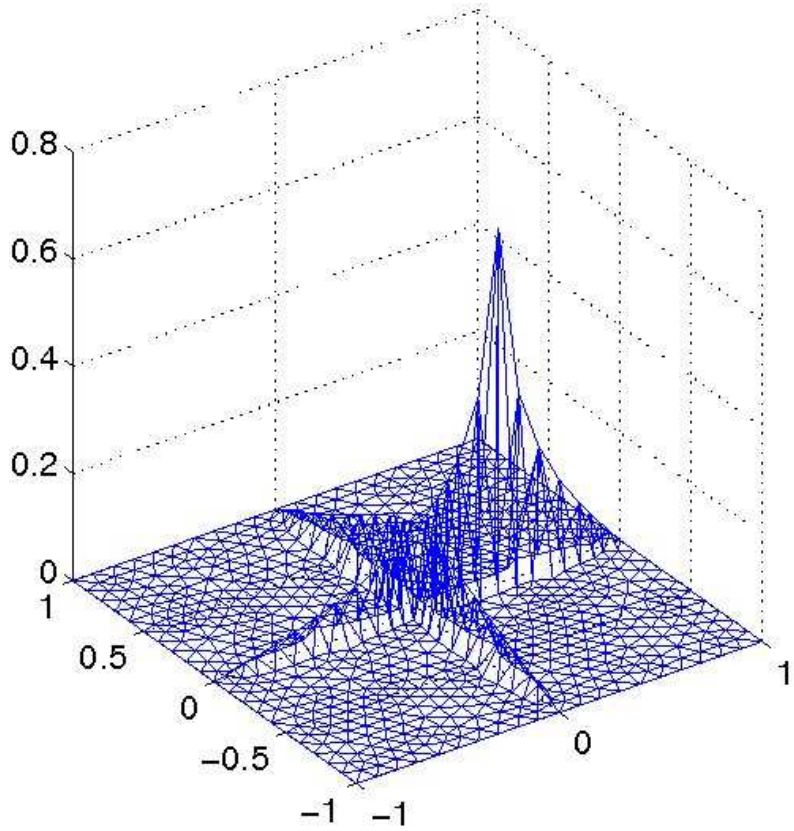
- QUANTUM graphs (metric graph)
- 2-D simplex
- Same theory with Laplace-Beltrami operator

Green functions on wirebasket

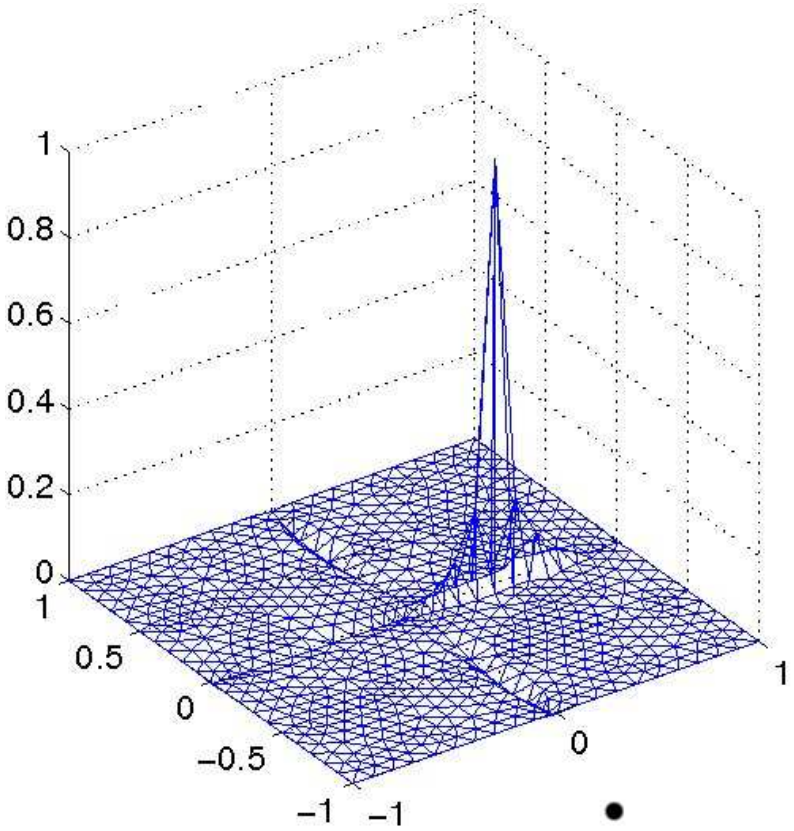


Steklov-Poincaré Green function

Green functions on wirebasket

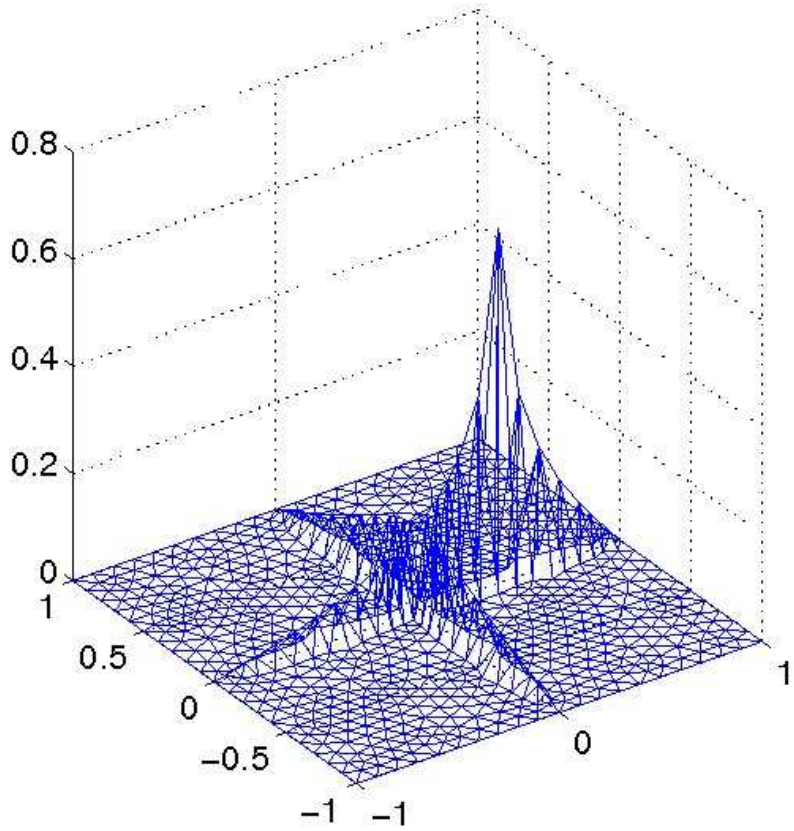


Steklov-Poincaré Green function

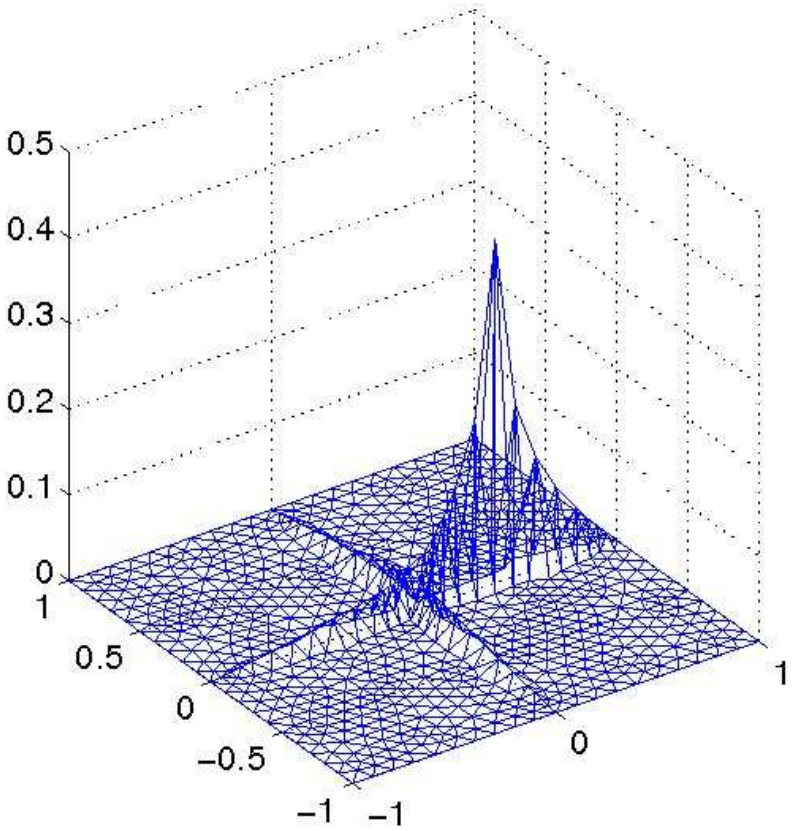


Neumann-Neumann Green function

Green functions on wirebasket



Steklov-Poincaré Green function



$H^{1/2}$ Green function

Open problems

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- Strange domains: 1D simplex (wirebasket) and QUANTUM GRAPH

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