Kernel-based Discretisation for Solving Matrix-valued PDEs

(based on work with Peter Giesl (Sussex))

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Contents

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Goal: Find M symmetric and positive definite, solving

$$Df^T(x)M(x) + M(x)Df(x) + M'(x) = -C(x), \qquad x \in \Omega.$$

Riemannian Contraction Metric

Consider $\dot{x} = f(x)$

Theorem

Let $\emptyset \neq G \subseteq \mathbb{R}^n$ be a compact, connected and positively invariant set and M be a Riemannian contraction metric in G, i.e.

- *$M \in C^1(G, \mathbb{R}^{n\times n})$, such that $M(x)$ is symmetric and positive definite for all $x \in G$.*
- *$Df(x)^T M(x) + M(x) Df(x) + M'(x)$ is negative definite for all $x \in G$.*

Then there exists one and only one equilibrium in x_0 in G; x_0 is exponentially stable and G is a subset of the basin of attraction $A(x_0)$.

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Definition

The Hilbert space $\mathcal{H}(\Omega; W)$ is called a reproducing kernel Hilbert space if there is a function $\Phi : \Omega \times \Omega \to \mathcal{L}(W)$ with

1. $\Phi(\cdot, x)\alpha \in \mathcal{H}(\Omega; W)$ for all $x \in \Omega$ and all $\alpha \in W$.
2. $\langle f(x), \alpha \rangle_W = \langle f, \Phi(\cdot, x)\alpha \rangle_{\mathcal{H}}$ for all $f \in \mathcal{H}(\Omega; W)$, all $x \in \Omega$ and all $\alpha \in W$.

The function Φ is called the reproducing kernel of $\mathcal{H}(\Omega; W)$.

Elementary Properties

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2. *The reproducing kernel satisfies* $\Phi(x, y)^* = \Phi(y, x)$ *for all* $x, y \in \Omega$.
3. *The reproducing kernel is positive semi-definite, i.e. it satisfies*

$$\sum_{i,j=1}^{N} \langle \alpha_i, \Phi(x_i, x_j)\alpha_j \rangle_W \geq 0$$

for all $x_1, \ldots, x_N \in \Omega$ *and all* $\alpha_1, \ldots, \alpha_N \in W$.

Interpolation

Theorem

If $x_1, \ldots, x_N$ are pairwise distinct points from Ω and if $f_1, \ldots, f_N \in W$ are given, then there is exactly one interpolant of the form

$$s_f(x) = \sum_{j=1}^{N} \Phi(x, x_j)\alpha_j$$

which satisfies $s_f(x_i) = f_i$, $1 \leq i \leq N$.

Generalised Interpolation

Theorem

Let H be a Hilbert space. Let $\lambda_1, \dots, \lambda_N \in H^*$ be linearly independent linear functionals with Riesz representers $v_1, \dots, v_N \in H$. Then the element $s^* \in H$ which solves

$$\min\{\|s\|_H : s \in H \text{ with } \lambda_j(s) = f_j, 1 \le j \le N\}$$

is given by

$$s^* = \sum_{k=1}^{N} \beta_k v_k,$$

where the coefficients are determined by $A_\Lambda \beta = f$ with the positive definite matrix $A_\Lambda = (a_{ik})$ having entries $a_{ik} = \lambda_i(v_k) = \langle v_k, v_i \rangle_H$.

Special Case

Theorem

Assume that $\{\alpha_j\}_{j\in J}$ is an orthonormal basis of W. Then, the Riesz representer of a functional $\lambda \in \mathcal{H}(\Omega; W)^*$ is given by

$$v_\lambda(x) = \sum_{j\in J} \lambda(\Phi(\cdot, x)\alpha_j)\alpha_j, \qquad x \in \Omega.$$

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$$v_\lambda(x) = \sum_{j\in J} \lambda(\Phi(\cdot, x)\alpha_j)\alpha_j, \qquad x \in \Omega.$$

$$s^* = \sum_{k=1}^{N} \beta_k \sum_{j\in J} \lambda_k^y(\Phi(y,\cdot)\alpha_j)\alpha_j,$$

the coefficients $\beta_k \in \mathbb{R}$ are determined by

$$\sum_{k=1}^{N} \lambda_i^x \left[\lambda_k^y \sum_{j\in J} (\Phi(y,x)\alpha_j)\,\alpha_j \right] \beta_k = f_i, \qquad 1 \le i \le N.$$

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A kernel Φ is now a mapping

$$\Phi : \Omega \times \Omega \to \mathcal{L}(\mathbb{R}^{n\times n}) \quad \text{or} \quad \Phi : \Omega \times \Omega \to \mathcal{L}(\mathbb{S}^{n\times n}),$$

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i.e. a tensor of order 4 represented as $\Phi = (\Phi_{ijk\ell})$ with

$$(\Phi(x,y)\alpha)_{ij} = \sum_{k,\ell=1}^{n} \Phi(x,y)_{ijk\ell}\alpha_{k\ell}, \qquad \alpha \in \mathbb{R}^{n\times n}(\mathbb{S}^{n\times n})$$

Sobolev Spaces

- $\mathcal{H}(\Omega, \mathbb{R}^{n\times n}) = H^\sigma(\Omega; \mathbb{R}^{n\times n})$ or $H^\sigma(\Omega; \mathbb{S}^{n\times n})$ component-wise.

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- Inner product:

$$\langle M, S\rangle_{H^\sigma(\Omega;\mathbb{R}^{n\times n})} := \sum_{i,j=1}^{n} \langle M_{ij}, S_{ij}\rangle_{H^\sigma(\Omega)};$$

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$$\langle M, S\rangle_{H^\sigma(\Omega;\mathbb{R}^{n\times n})} := \sum_{i,j=1}^{n} \langle M_{ij}, S_{ij}\rangle_{H^\sigma(\Omega)};$$

- Reproducing kernel: Let $\phi : \Omega \times \Omega \to \mathbb{R}$ be a reproducing kernel of $H^\sigma(\Omega)$ and set

$$\Phi(x,y)_{ijk\ell} := \phi(x,y)\delta_{ik}\delta_{j\ell}, \qquad x, y \in \Omega, 1 \le i, j, k, \ell \le n.$$

Main Result

Theorem

$\Omega \subseteq \mathbb{R}^d$ bounded, Lipschitz. $\sigma, \tau > d/2$. Let $F : H^\sigma(\Omega; \mathbb{R}^{n\times n}) \to H^\tau(\Omega; \mathbb{R}^{n\times n})$ ($F : H^\sigma(\Omega; \mathbb{S}^{n\times n}) \to H^\tau(\Omega; \mathbb{S}^{n\times n})$) be linear and bounded. Finally, let $X = \{x_1, \dots, x_N\} \subseteq \Omega$ be given and let

$$\lambda_k^{(i,j)}(M) := e_i^T F(M)(x_k) e_j, \qquad 1 \le k \le N, \quad {}_{1\le i\le j\le n}^{1\le i,j\le n}.$$

Then each $\lambda_k^{(i,j)}$ belongs to the dual of $H^\sigma(\Omega; \mathbb{R}^{n\times n})$ ($H^\sigma(\Omega; \mathbb{S}^{n\times n})$). If they are linearly independent and if S denotes the optimal recovery of $M \in H^\sigma(\Omega; \mathbb{R}^{n\times n})$ ($H^\sigma(\Omega; \mathbb{S}^{n\times n})$) then

$$\|F(M) - F(S)\|_{L_\infty(\Omega;\mathbb{R}^{n\times n})} \le C h_{X,\Omega}^{\tau - d/2} \|M\|_{H^\sigma(\Omega;\mathbb{R}^{n\times n})}.$$

Contraction Metric

$$F(M)(x) := Df^T(x)M(x) + M(x)Df(x) + \nabla M(x)\cdot f(x) = -C. \quad (1)$$

Theorem

$f \in C^{\lceil\sigma\rceil}(\mathbb{R}^n;\mathbb{R}^n)$, $\sigma > n/2+1$. Let x_0 be an exponentially stable equilibrium of $\dot{x} = f(x)$ with basin of attraction $A(x_0)$. Let $C \in \mathbb{S}^{n\times n}$ be a positive definite (constant) matrix and let $M \in C^\sigma(A(x_0),\mathbb{S}^{n\times n})$ be the solution of (1). Let $K \subseteq \Omega \subseteq A(x_0)$ be a positively invariant and compact set, where Ω is open with Lipschitz boundary. Finally, let S be the optimal recovery. Then,

$$\begin{aligned}\|M-S\|_{L_\infty(K;\mathbb{S}^{n\times n})} &\leq c\|F(M)-F(S)\|_{L_\infty(\Omega;\mathbb{S}^{n\times n})}\\ &\leq Ch_{X,\Omega}^{\sigma-1-n/2}\|M\|_{H^\sigma(\Omega;\mathbb{S}^{n\times n})}.\end{aligned}$$

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- The system:

$$\dot{x} = -x + y, \qquad \dot{y} = x - 2y,$$

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- The RBF:

$$\phi(r) = (1 - cr)^{10}(2145(cr)^4 + 2250(cr)^3 + 1050(cr)^2 + 250cr + 25)_+$$

with $c = 0.9$ which is a reproducing kernel in $H^\sigma(\mathbb{R}^2)$ with $\sigma = 5.5$.

Errors

$X_\alpha = \{(x, y) \in \mathbb{R}^2 : x, y = -1, \dots, -2\alpha, -\alpha, 0, \alpha, 2\alpha, \dots, 1\}$ with $\alpha = 1, \frac{1}{2}, \frac{1}{2^2}, \dots, \frac{1}{2^5}$.

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$$\begin{aligned} e_\alpha &= \max_{x \in X_{check}} \|S^\alpha(x) - M(x)\|_{\max} = \max_{x \in X_{check}} \max_{i,j=1,2} |S^\alpha_{ij}(x) - M_{ij}(x)| \\ e^s_\alpha &= \max_{x \in X_{check}} \|F(S^\alpha)(x) - F(M)(x)\|_{\max}, \end{aligned}$$

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α	e^s_α	$e^s_{2\alpha}/e^s_\alpha$	e_α	$e_{2\alpha}/e_\alpha$
1/2	2.5724		1.2334	
1/4	1.2833	2.0045	0.9169	1.3452
1/8	0.3516	3.6499	0.0124	73.9435
1/16	0.0329	10.6838	5.6040e-4	22.1271
1/32	0.0025	13.1918	1.6311e-5	34.3572
$2^{3.5}$		11.3137		11.3137

Pictures

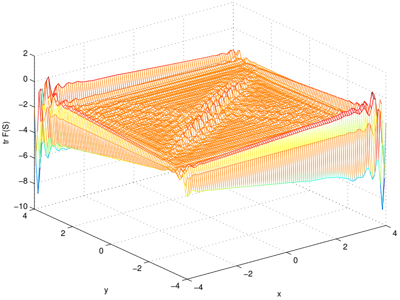

Figure: Left: trace $F(S)(x, y)$, right: $-\det F(S)(x, y)$. If both functions are negative, then $F(S)(x, y)$ is negative definite.

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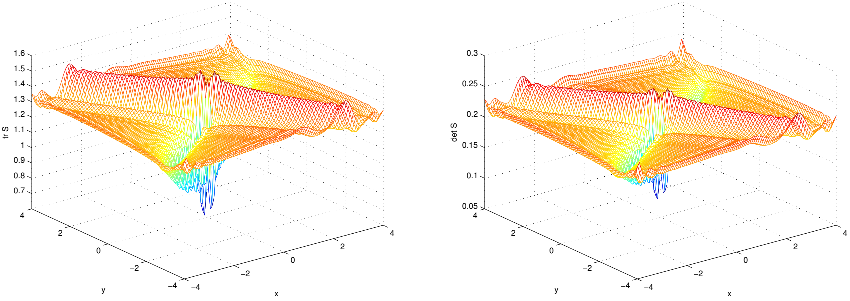

Figure: Left: trace$S(x, y)$, right: $\det S(x, y)$. If both functions are positive, then $S(x, y)$ is positive definite.

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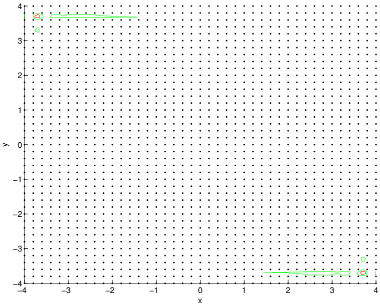

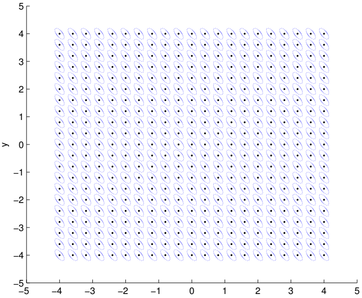

Figure: Left: Points used for RBF approximation and areas where trace $F(S)(x,y) = 0$ (red) and det $F(S)(x,y) = 0$ (green). Right: We have plotted the curve of equal distance with respect to metric $S(\mathbf{x})$, in particular the set $\{\mathbf{x}+\mathbf{v} \mid (\mathbf{v}-\mathbf{x})^T S(\mathbf{x})(\mathbf{v}-\mathbf{x}) = \text{const}\}$.