The dimension weighted fast multipole method for scattered data approximation

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Outline

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4. The dimension weighted fast multipole method
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Harbrecht et al. 2016

Problem formulation

- We consider the following stationary diffusion problem

$$-\Delta u(\omega) = f \text{ in } D(\omega), \quad u(\omega) = 0 \text{ on } \partial D(\omega), \quad \omega \in \Omega,$$

for an uncertain domain $D(\omega) \subset \mathbb{R}^N$.

- We denote by $D_0 \subset \mathbb{R}^D$, for $d \in \mathbb{N}$, a domain with Lipschitz continuous boundary.
- To model the shape uncertainty, we introduce a random deformation field $\boldsymbol{\chi}\colon D_0 \times \Omega \to \mathbb{R}^n$.
- We impose the uniformity condition

$$\|\boldsymbol{\chi}(\omega)\|_{C^1(\overline{D_0};\mathbb{R}^n)}, \|\boldsymbol{\chi}^{-1}(\omega)\|_{C^1(\overline{D(\omega)};\mathbb{R}^n)} \lesssim 1 \quad \text{for } \mathbb{P}\text{-a.e. } \omega \in \Omega,$$

which satisfies

$$D(\omega) = \boldsymbol{\chi}(D_0, \omega).$$

- We consider the Karhunen-Loève expansion

$$\chi(\omega) = \mathrm{Id} + \sum_{k=1}^{M} \sigma_k \chi_k Y_k(\omega), \quad \omega \in \Omega.$$

- $\{Y_k\}$ are i.i.d. random variables uniformly distributed on $[-1, 1]$.
- Parametrizing the random variable by their image, we obtain the parametric deformation field

$$\chi(\zeta) = \mathrm{Id} + \sum_{k=1}^{M} \sigma_k \chi_k \zeta_k, \quad \zeta \in [-1, 1]^M. \tag{1}$$

- We have now a parametric diffusion problem

$$-\Delta u(\zeta) = f \text{ in } D(\zeta), \quad u(\zeta) = 0 \text{ on } \partial D(\zeta), \quad \zeta \in [-1, 1]^M.$$

- The goal we consider consists of the solution-based functional reconstruction:

$$F(u)(\zeta) = \left(u \circ \boldsymbol{\chi}^{-1}(\zeta), \phi\right)_{L^2(D_0)}. \tag{2}$$

- Each ζ_k in (1) introduces additional dimensions to the problem.
- The importance of each dimension is weighted by σ_k, which decays as k increases, creating anisotropic data.
- To reconstruct the quantity of interest we use the fast anisotropic kernel method.
- **Goal**: Given functional observed values $\boldsymbol{F}$, we want to solve $\boldsymbol{K}\boldsymbol{\alpha} = \boldsymbol{F}$, where $\boldsymbol{K}$ representes the kernel matrix associated with the interpolation problem.

Kernels on anisotropic data sets

Definition. Let $\Omega \subset \mathbb{R}^d$ and $\big(\mathcal{H}, (\cdot,\cdot)_\mathcal{H}\big)$ be a Hilbert space of functions $h\colon \Omega \to \mathbb{R}$. A *reproducing kernel* $\mathcal{K}$ for $\mathcal{H}$ is a function $\mathcal{K} : \Omega \times \Omega \to \mathbb{R}$ such that

1. $\mathcal{K}(\cdot, \boldsymbol{x}) \in \mathcal{H}$ for all $\boldsymbol{x} \in \Omega$,
2. $h(\boldsymbol{x}) = \big(h, \mathcal{K}(\cdot, \boldsymbol{x})\big)_\mathcal{H}$ for all $h \in \mathcal{H}$ and all $\boldsymbol{x} \in \Omega$.

If $\mathcal{H}$ exhibits a reproducing kernel, we call it a *reproducing kernel Hilbert space (RKHS)*.

- Given a set of *data sites* $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \mathbb{R}^d$ and *data values* $F_1, \dots, F_N \in \mathbb{R}$, we may want to solve the kernel ridge regression

$$\min_{\alpha_1,\dots,\alpha_N} \sum_{i=1^n} \big(F_i - s_X(\boldsymbol{x}_i)\big)^2 + \lambda \|s_X\|_\mathcal{H}^2 \to (\boldsymbol{K} + \lambda \boldsymbol{I})\boldsymbol{\alpha} = \boldsymbol{F},$$

where $s_X(\boldsymbol{x}) = \sum_{i=1}^N \alpha_i \, \mathcal{K}(\boldsymbol{x}, \boldsymbol{x}_i)$ is the kernel interpolant.

- **Problem:** Direct computation of all pairwise interactions for large N is costly.
- To compress $\boldsymbol{K}$, we exploit kernel expansions obtained by interpolation.
- In particular, to deal with posssibly high dimensional data, we use interpolation by anistropic total degree polynomials.

Definition. The data set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \Omega$ is quasi-uniform if the *fill distance*

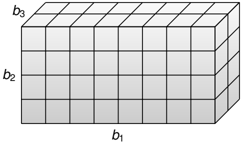
$$h_{X,\Omega} := \sup_{\boldsymbol{x}\in\Omega} \min_{\boldsymbol{x}_i \in X} \|\boldsymbol{x} - \boldsymbol{x}_i\|_2$$

is proportional to the separation radius $q_X := \min_{i\neq j} \|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2$, i.e., there exists a constant $c_{X,\Omega} \in (0,1)$ such that $0 < c_{X,\Omega} \leq \frac{q_X}{h_{X,\Omega}} \leq \frac{1}{c_{X,\Omega}}$.

- We assume that the set X is *quasi-uniform* and contained in an anisotropic axis parallel cuboid

$$\mathcal{B} = [0, b_1] \times \cdots \times [0, b_d],$$

with *dimension weights* $b_1 \geq \ldots \geq b_d \geq 0$.



In this framework, the first step is to show the existence of an analytic extension of the kernel function:

- We introduce the linear transformation

$$\boldsymbol{B}\colon [0,1]^d \to \mathcal{B}, \quad \hat{\boldsymbol{x}} \mapsto \boldsymbol{x} = \boldsymbol{B}\hat{\boldsymbol{x}},$$

  which is given by the matrix $\boldsymbol{B} := \mathrm{diag}(b_1, \ldots, b_d)$.
- Thus, considering the kernel $\mathcal{K}\colon \mathcal{B} \times \mathcal{B} \to \mathbb{R}$ yields to the *transported kernel*

$$\mathcal{K}_{\boldsymbol{B}}\colon [0,1]^d \times [0,1]^d \to \mathbb{R}, \quad \mathcal{K}_{\boldsymbol{B}}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}) := \mathcal{K}(\boldsymbol{B}\hat{\boldsymbol{x}}, \boldsymbol{B}\hat{\boldsymbol{y}}). \tag{3}$$

- The analysis of the kernel interpolation is based on the *asymptotical smoothness* property of the kernel $\mathcal{K}$, that is

$$\left|\frac{\partial^{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|}}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}} \partial \boldsymbol{y}^{\boldsymbol{\beta}}} \mathcal{K}(\boldsymbol{x}, \boldsymbol{y})\right| \leq c_{\mathcal{K}} \frac{(|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|)!}{\rho^{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|}\|\boldsymbol{x}-\boldsymbol{y}\|_2^{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|}}, \quad c_{\mathcal{K}}, \rho > 0. \tag{4}$$

- The derivatives of the transported kernel satisfy the bound

$$\left|\frac{\partial^{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|}}{\partial \hat{\boldsymbol{x}}^{\boldsymbol{\alpha}} \partial \hat{\boldsymbol{y}}^{\boldsymbol{\beta}}} \mathcal{K}_{\boldsymbol{B}}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}})\right| \leq c_{\mathcal{K}} \left(\frac{\boldsymbol{b}}{\rho}\right)^{\boldsymbol{\alpha}+\boldsymbol{\beta}} \frac{(|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|)!}{\|\boldsymbol{B}(\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}})\|_2^{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|}},$$

with $\boldsymbol{b} := [b_1 \ldots, b_d]$.

- Inserting a lower bound $\eta > 0$ for the distance of now yields the analyticity of the transported kernel for any pair of points $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}} \in [0,1]^d$ satisfying $\|\boldsymbol{B}(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}})\|_2 \geq \eta$.

Corollary. Let $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}} \in [0,1]^d$ be such that $\|\boldsymbol{B}(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}})\|_2 \geq \eta$ for some $\eta > 0$. Then, each component of the kernel function $\mathcal{K}_{\boldsymbol{B}}$ from (3) admits an analytic extension into $\boldsymbol{\Sigma}(\boldsymbol{\tau})$ for $\tau_k \in [0, c_k \eta \rho / b_k]$, where $c_k > 0$ and $\gamma := \sum_{k=1}^{d} c_k < 1$, where $\boldsymbol{\Sigma}(\boldsymbol{\tau}) := \Sigma(\tau_1) \times \cdots \times \Sigma(\tau_d)$ with $\Sigma(\tau) := \{z \in \mathbb{C} : \mathrm{dist}(z, [0,1]) \leq \tau\}$.

DeVore and Lorentz 1993

Weighted total degree polynomial approximation

- Exploiting the available anisotropy for approximation, we derive corresponding estimates of the error for polynomial best approximation and extend them to the interpolation case.

Lemma. Let $\Pi_q := \operatorname{span}\{1, \ldots, x^q\}$ denote the space of all univariate polynomials up to degree q. Given a function $f \in C([0,1])$ which admits an analytic extension $\tilde{f}$ into the region $\Sigma(\tau)$ for some $\tau > 0$, there holds, for $1 < \rho := 2\tau + \sqrt{1 + 4\tau^2}$, that

$$\min_{w \in \Pi_q} \|f - w\|_{C([0,1])} \leq \frac{2\rho}{\rho - 1} e^{-(q+1)\log\rho} \|\tilde{f}\|_{C(\Sigma(\tau))}.$$

- We therefore define the projection operator

$$U_q\colon C([0,1]) \to \Pi_q, \quad U_q f := \operatorname{argmin}_{w\in\Pi_q} \|f - w\|_{C([0,1])}.$$

- By observing $(U_0 f)(x) = \frac{1}{2}\bigg(\min_{y\in[0,1]} f(y) + \max_{y\in[0,1]} f(y)\bigg)$, we infer the stability estimate

$$\|U_0 f\|_{C([0,1])} \leq \|f\|_{C([0,1])}.$$

- To define the weighted total degree approximation, we introduce the *weighted total degree index sets*

$$\Lambda_{\boldsymbol{\omega},q,d} := \bigg\{\mathbf{0} \leq \boldsymbol{\alpha} \in \mathbb{N}^d : \sum_{\ell=1}^{d} \omega_\ell \alpha_\ell \leq q\bigg\}, \boldsymbol{\omega} \in [0,\infty)^d.$$

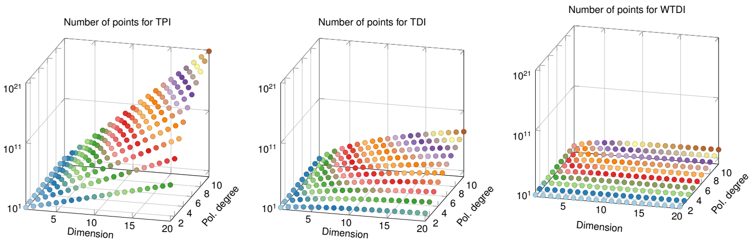


Figure: Number of interpolation points required for TPI, TDI, and WTDI based on a quadratic increase of the sequence $\{\tau_k\}$ of the convergence radii.

- Given the index set $\Lambda_{\boldsymbol{\omega},q,d}$, we define

$$\mathcal{P}_{\boldsymbol{\omega},q} := \operatorname{span}\{\boldsymbol{x}^{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \Lambda_{\boldsymbol{\omega},q,d}\}.$$

- With respect to $\mathcal{P}_{\boldsymbol{\omega},q}$, we introduce the *weighted total degree approximation operator of degree* $q \in \mathbb{N}$ given by

$$P_{\boldsymbol{\omega},q} \colon C([0,1]^d) \to \mathcal{P}_{\boldsymbol{\omega},q}, \quad P_{\boldsymbol{\omega},q} f := \sum_{\boldsymbol{\alpha} \in \Lambda_{\boldsymbol{\omega},q,d}} \Delta_{\boldsymbol{\alpha}} f.$$

Harbrecht et al. 2024; Haji-Ali et al. 2018

Theorem. Let $v \in C([0,1]^d)$ admit an analytic extension $\tilde{v}$ into the region $\boldsymbol{\Sigma}(\boldsymbol{\tau})$ for a monotonously increasing sequence $0 < \tau_1 \leq \ldots \leq \tau_d \leq \ldots$ and $\tau_k \geq ck^r$ for some $c, r > 1$. Define $1 < \rho_k := 2\tau_k + \sqrt{1 + 4\tau_k^2}$ for $k = 1, \ldots, d$ and introduce the weights $\omega_k := \log \rho_k$. Then, there holds

$$\left\|(\mathrm{Id}^{(d)} - P_{\boldsymbol{\omega},q})v\right\|_{C([0,1]^d)} \leq c_r 2^{d+1} e^{-q(1-\frac{1}{r}\log\log d)} \|\tilde{v}\|_{C(\boldsymbol{\Sigma}(\boldsymbol{\tau}))}$$

with the constant c_r such that $|\Lambda_{\boldsymbol{\omega},q,d}| \leq c_r \log(d)^{\frac{q}{r}}$.

Corollary. Under the same hypotheses, there holds for the interpolation $I_{\boldsymbol{\omega},q}\colon C([0,1]^d) \to \mathcal{P}_{\boldsymbol{\omega},q}$ with Lebesgue constant $L_{\boldsymbol{\omega},q}$ that

$$\left\|(\mathrm{Id}^{(d)} - I_{\boldsymbol{\omega},q})v\right\|_{C([0,1]^d)} \leq (1 + L_{\boldsymbol{\omega},q}) c_r 2^{d+1} e^{-q(1-\frac{1}{r}\log\log d)} \|\tilde{v}\|_{C(\boldsymbol{\Sigma}(\boldsymbol{\tau}))}.$$

The dimension weighted fast multipole method

- We provide a cardinality balanced clustering for set of data sites X which yields a balanced binary tree $\mathcal{T}$.
- The clusters $\nu, \nu' \in \mathcal{T}$ with $j_\nu = j_{\nu'}$ are called *admissible* iff

$$\operatorname{dist}(B_\nu, B'_\nu) \geq \eta \max \left\{ \operatorname{diam} B_\nu, \operatorname{diam} B'_\nu \right\}$$

  holds for some $\eta > 0$.
- We denote by

$$\mathcal{T} \boxtimes \mathcal{T} := \{\nu \times \nu' \colon \nu, \nu' \in \mathcal{T},\ j_\nu = j'_\nu\}$$

  the level-wise Cartesian product of the cluster tree $\mathcal{T}$,

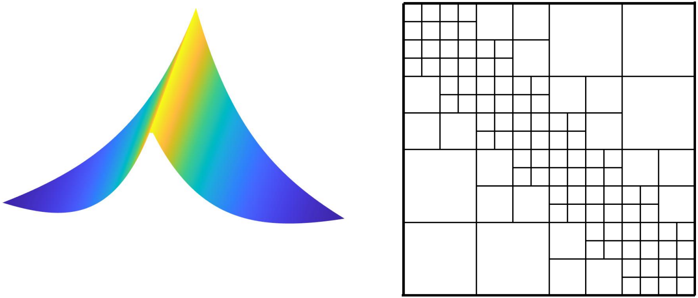


Figure: $\mathcal{H}^2$-*matrices* formalise a certain class of matrices, which exhibit a low-rank structure with respect to a given block-clustering.

- Given an admissible cluster $\nu \times \nu'$, we now approximate

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) \approx \widetilde{\mathcal{K}}(\boldsymbol{x}, \boldsymbol{y}) := \sum_{\boldsymbol{\alpha}, \boldsymbol{\alpha}' \in X_{\boldsymbol{\omega}, q, d}} c_{\boldsymbol{\alpha}, \boldsymbol{\alpha}'}^{\nu, \nu'} p_{\boldsymbol{\alpha}}^{\nu}(\boldsymbol{x}) p_{\boldsymbol{\alpha}'}^{\nu'}(\boldsymbol{y})$$

with coefficients $c_{\boldsymbol{\alpha}, \boldsymbol{\alpha}'}^{\nu, \nu'} \in \mathbb{R}$ and the transported polynomials

$$p_{\boldsymbol{\alpha}}^{\nu} := \hat{p}_{\boldsymbol{\alpha}} \circ a_{\nu}^{-1}.$$

- The coefficients $c_{\boldsymbol{\alpha}, \boldsymbol{\alpha}'}^{\nu, \nu'}$ in matrix notation according to

$$\boldsymbol{C}_{\nu, \nu'} := [c_{\boldsymbol{\alpha}, \boldsymbol{\alpha}'}^{\nu, \nu'}]_{\boldsymbol{\alpha}, \boldsymbol{\alpha}' \in \Lambda_{\boldsymbol{\omega}, q, d}} = \boldsymbol{V}^{-1} \boldsymbol{S}_{\nu, \nu'} \boldsymbol{V}^{-\intercal}.$$

- The coupling matrix is

$$\boldsymbol{S}_{\nu, \nu'} := \left[\mathcal{K}\big(a_{\nu}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}}), a_{\nu'}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'})\big)\right]_{\boldsymbol{\alpha}, \boldsymbol{\alpha}' \in \Lambda_{\boldsymbol{\omega}, q, d}}.$$

Börm 2010

- We approximate the matrix block $\boldsymbol{K}_{\nu,\nu'}$ as:

$$\boldsymbol{K}_{\nu,\nu'} \approx \widetilde{\boldsymbol{K}}_{\nu,\nu'} = \boldsymbol{P}_{\nu} \boldsymbol{C}_{\nu,\nu'} \boldsymbol{P}_{\nu'}^{\mathsf{T}} = \boldsymbol{P}_{\nu} \boldsymbol{V}^{-1} \boldsymbol{S}_{\nu,\nu'} \boldsymbol{V}^{-\mathsf{T}} \boldsymbol{P}_{\nu'}^{\mathsf{T}}.$$

- By fixing the index set $\Lambda_{\boldsymbol{\omega},q,d}$ for all clusters,

$$\boldsymbol{T}_{\nu_{\text{child}}} := \boldsymbol{V}^{-1} \left[p_{\boldsymbol{\alpha}'}^{\nu} \left(a_{\nu_{\text{child}}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}}) \right) \right]_{\boldsymbol{\alpha},\boldsymbol{\alpha}' \in \Lambda_{\boldsymbol{\omega},q,d}},$$

  there holds the two-scale relation

$$\boldsymbol{P}_{\nu} = \begin{bmatrix} \boldsymbol{P}_{\nu_{\text{child}_1}} \boldsymbol{T}_{\nu_{\text{child}_1}} \\ \boldsymbol{P}_{\nu_{\text{child}_2}} \boldsymbol{T}_{\nu_{\text{child}_2}} \end{bmatrix}.$$

Lemma. Let the assumptions of the previous Theorem be satisfied for $\tau_k \in [0, c_k\eta\rho/b_k]$. In case of quasi-uniform points, the matrix $\widetilde{\boldsymbol{K}}$ satisfies the following error estimate

$$\frac{\big\|\boldsymbol{K} - \widetilde{\boldsymbol{K}}\big\|_F}{\big\|\boldsymbol{K}\big\|_F} \lesssim (1 + L_{\boldsymbol{\omega},q})c_r 2^d e^{-q(1-\frac{1}{r}\log\log d)} \frac{c_{\mathcal{K}}}{1-\gamma}.$$

Numerical results

- The reference shape D_0 is given by the kite domain shown in this figure with bounding box $[-0.26, 0.39] \times [-0.39, 0.39]$. It is discretized by 327 680 piecewise linear parametric finite elements.

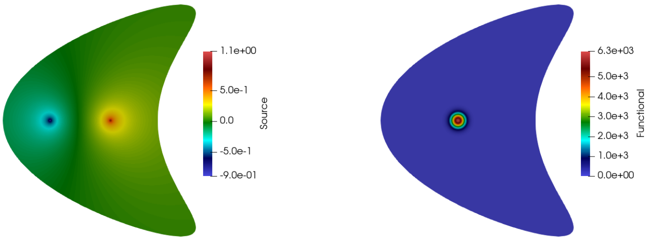


Figure: Visualization of the source term (left) and the functional ϕ (right).

- In order to define the deformation field, we compute the first 20 eigenfunctions $\{\chi_k\}$ of the matrix-valued covariance kernel

$$\mathcal{C}\colon D_0 \times D_0 \to \mathbb{R}^{2\times 2}, \quad \mathcal{C}(\boldsymbol{x}, \boldsymbol{y}) := \begin{bmatrix} 10^2 e^{-5\|\boldsymbol{x}-\boldsymbol{y}\|_2^2} & e^{-\|\boldsymbol{x}-\boldsymbol{y}\|_2^2} \\ e^{-\|\boldsymbol{x}-\boldsymbol{y}\|_2^2} & 10^2 e^{-5\|\boldsymbol{x}-\boldsymbol{y}\|_2^2}, \end{bmatrix}$$

  discretized on the aforementioned finite element mesh.

- The singular values are set to be $\sigma_k := 0.25k^{-3}$.

- We consider the source term

$$f(\boldsymbol{x}) = \frac{1}{2\pi}\big(\log\|\boldsymbol{x}+\boldsymbol{x}_0\|_2 - \log\|\boldsymbol{x}-\boldsymbol{x}_0\|_2\big), \quad \boldsymbol{x} \in \mathbb{R}^2,$$

  where $\boldsymbol{x}_0 = [0.1, 0]^\intercal \in D_0$.

- The particular quantity of interest (2) involves the localized Gaussian

$$\phi(\boldsymbol{x}) = \frac{5\pi}{10^4} e^{-\frac{5}{10^4}\|\boldsymbol{x}\|_2^2}.$$

- We consider $N = 849\,375$ data points for the kernel interpolation, obtained by rescaling each component of the Monte Carlo samples $\boldsymbol{\zeta}_1, \ldots, \boldsymbol{\zeta}_N$ by the respective singular value, i.e., $x_{i,k} = \sigma_k \zeta_{i,k}$, resulting in points $\boldsymbol{x}_1, \ldots \boldsymbol{x}_N \in \times_{k=1}^{M} [-\sigma_k, \sigma_k]$.
- These points are then shifted by the choice $b_k = 2\sigma_k$ for all $k = 1, \ldots, N$ such that $X \in \mathcal{B}$.
- We perform a dimension truncation with a relative error of 10^{-3}, resulting in $d = 20$ dimensions.
- We apply the exponential kernel $\mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) = \exp(\|\boldsymbol{x} - \boldsymbol{y}\|_2/\sigma)$.

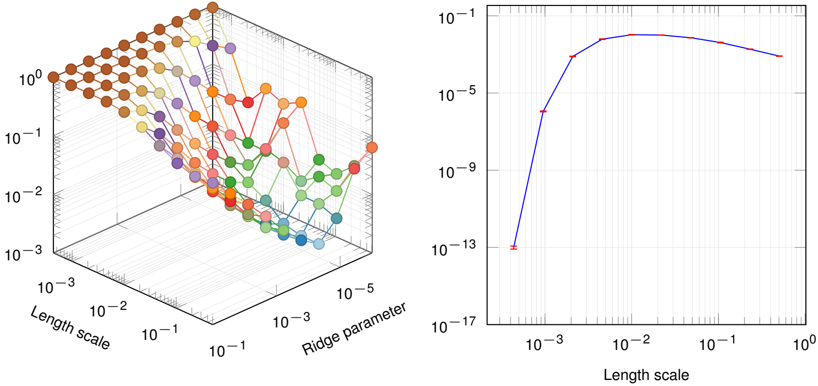


Figure: Average prediction error (left) and compression error in blue with its standard variation in red (right).

Thank you

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