High-dimensional Approximation: Transforming periodic Approximation vs. Random Fourier Features

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joint work with Daniel Potts, Tino Ullrich and Rachel Ward

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Applied Functional Analysis

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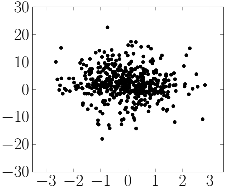
Given data

- sample points $\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^d$ with $|\mathcal{X}| = M$, i.i.d. according to density $\mu\colon \mathbb{R}^d \to \mathbb{R}_+$
- function values $\boldsymbol{f} = (f(\boldsymbol{x}))_{\boldsymbol{x}\in\mathcal{X}}$



Aim

Approximate the function $f\colon \mathbb{R}^d \to \mathbb{C}$

Trafo approach

- transform the samples to the torus $\mathbb{T}^d = [-\frac{1}{2}, \frac{1}{2})^d$
- use approximation operator on $\mathbb{T}^d$

Random Fourier Features

- draw frequencies $\omega_j \in \mathbb{R}^d$ at random
- $f(\cdot) \approx \sum_j a_j \mathrm{e}^{\mathrm{i}\langle \omega_j, \cdot\rangle}$

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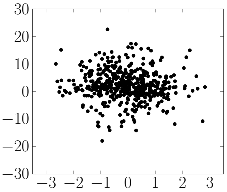

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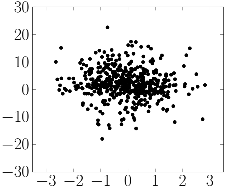

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Outline

1. Approximation of periodic function
2. Variable Transformations
3. Approximation results on $\mathbb{R}^d$
4. Random Fourier Features
5. ANOVA decomposition

L. Lippert, D.Potts, T. Ullrich
Fast Hyperbolic Wavelet Regression meets ANOVA
Numer. Math. 154, 155-207 (2023)

L. Lippert, D.Potts
Variable Transformations in combination with Wavelets and ANOVA for high-dimensional approximation
arXiv:2108.13197, 2022

Approximation of periodic functions

given data: samples $\mathcal{X} \subset \mathbb{T}^d$, $|\mathcal{X}| = M$, function values $\boldsymbol{f} = (f(\boldsymbol{x}))_{\boldsymbol{x}\in\mathcal{X}}$

procedure:

- choose basis functions: $\psi^{\mathrm{per}}_{\boldsymbol{j},\boldsymbol{k}}(x)$ (periodized Chui-Wang wavelets of order m)
- also other basis functions are possible, e.g. $\mathrm{e}^{\mathrm{i}\langle \boldsymbol{k},\boldsymbol{x}\rangle}, \cos(\langle \boldsymbol{k},\boldsymbol{x}\rangle), \dots$
- use index-set $(\boldsymbol{j},\boldsymbol{k}) \in I_n$ with $N := |I_n| = \mathcal{O}(2^n n^{d-1})$
- choose wavelet level n according to logarithmic oversampling $M \gtrsim N \log N$
- solve minimizing problem iteratively:

$$\boldsymbol{a} = \operatorname{argmin} \|\boldsymbol{A}\boldsymbol{a} - \boldsymbol{f}\|_2\,, \quad \boldsymbol{A} = \left(\psi^{\mathrm{per}}_{\boldsymbol{j},\boldsymbol{k}}(\boldsymbol{x})\right)_{\boldsymbol{x}\in\mathcal{X},(\boldsymbol{j},\boldsymbol{k})\in I_n} \in \mathbb{R}^{M\times N}$$

- construct approximant

$$S_n^{\mathcal{X}} f(\boldsymbol{x}) := \sum_{(\boldsymbol{j},\boldsymbol{k})\in I_n} a_{\boldsymbol{j},\boldsymbol{k}} \psi^{\mathrm{per}}_{\boldsymbol{j},\boldsymbol{k}}(\boldsymbol{x})$$

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Theorem ([L., Potts, Ullrich, '23])

Let $\mathcal{X} \sim$ *i.i.d. uniformly,* $M \geq r\, N \log N$, m *the order of the wavelets, if* $\frac{1}{2} < s < m$:

$$\mathbb{P}\left(\left\|f - S_n^{\mathcal{X}} f\right\|_{L_2(\mathbb{T}^d)} \lesssim 2^{-ns} n^{(d-1)/2} \, \|f\|_{\boldsymbol{B}^s_{2,\infty}(\mathbb{T}^d)}\right) \geq 1 - 2\, M^{-r}.$$

and if $m = s$

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important assumptions:

- uniformly distributed samples with $M \gtrsim N \log N$, ($N \sim 2^n n^{d-1}$)
- regularity of the function: $f \in H^s_{\mathrm{mix}}(\mathbb{T}^d)$ or $f \in \boldsymbol{B}^s_{2,\infty}(\mathbb{T}^d)$

result: error decay $\sim N^{-s} (\log N)^{(s+1/2)(d-1)}$

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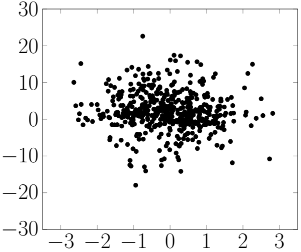
Constructing the transformation

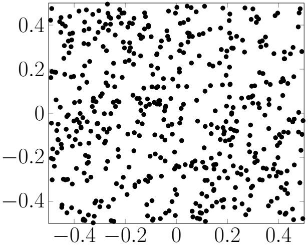
$\mathbb{R}^d$



samples $\mathcal{X}$

$\xrightarrow{\mathrm{R}}$

$\mathbb{T}^d$



transformed samples $\mathcal{Y}$

one-dimensional case:

$$\mathrm{R}\colon \mathbb{R} \to [-\tfrac{1}{2}, \tfrac{1}{2}], \quad \mathrm{R}(x) := \int_{-\infty}^{x} \mu(t)\mathrm{d}t - \tfrac{1}{2}$$

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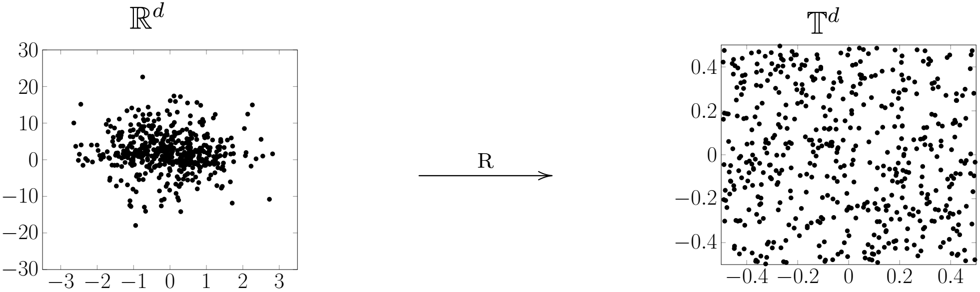

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multi-dimensional case

assumptions:

- independent input variables, i.e. $\mu(\boldsymbol{x}) = \prod_{i=1}^{d} \mu_i(x_i)$

$\rightarrow$ transform every dimension separately:

$$\mathrm{R}(\boldsymbol{x}) := (\mathrm{R}_1(x_1), \dots, \mathrm{R}_d(x_d))$$

useful properties of the transformation

- there exists an inverse

$$\mathrm{R}^{-1}(\boldsymbol{y}) := (\mathrm{R}_1^{-1}(y_1), \dots, \mathrm{R}_d^{-1}(y_d))$$

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- transform samples $\mathcal{Y} = \mathrm{R}(\mathcal{X})$
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$$
\begin{tikzcd}
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$$\left(S_n^{\mathcal{Y}}(f \circ \mathrm{R}^{-1})\right) \circ \mathrm{R}$$

preservation of L_2-norm:

$$\|f\|_{L_2(\mathbb{R}^d,\mu)}^2 := \int_{\mathbb{R}^d} |f(\boldsymbol{x})|^2 \mu(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \|f \circ \mathrm{R}^{-1}\|_{L_2(\mathbb{T}^d)}^2$$

$\rightarrow$ measure error in $\|\cdot\|_{L_2(\mathbb{R}^d,\mu)}$

idea:

introduce function spaces $H_{\mathrm{mix}}^m(\mathbb{R}^d,\mu)$ with $\|f \circ \mathrm{R}^{-1}\|_{H_{\mathrm{mix}}^m(\mathbb{T}^d)} = \|f\|_{H_{\mathrm{mix}}^m(\mathbb{R}^d,\mu)}$

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Weighted function spaces (one-dimensional)

Weighted Sobolev norms on $\mathbb{R}$:

$$\|f\|^2_{H^m(\mathbb{R},\mu)} := \sum_{k=0}^{m} \left\|\mathrm{D}^k f\right\|^2_{L_2(\mathbb{R},\Upsilon_{m,k})} \text{ with } \Upsilon_{m,k}(x) := \begin{cases} \sum_{\alpha=k}^{m} |B_{\alpha,k}(x)|^2 \mu(x) & \text{if } 1 \leq k \leq m, \\ \mu(x) & \text{if } k = 0. \end{cases}$$

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Examples:

$$\|f\|^2_{H^0(\mathbb{R},\mu)} = \|f\|^2_{L_2(\mathbb{R},\mu)} = \left\|f \circ \mathrm{R}^{-1}\right\|^2_{H^0(\mathbb{T}^d)}$$

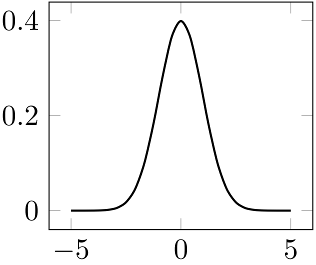
$$\|f\|^2_{H^1(\mathbb{R},\mu)} = \|f\|^2_{L_2(\mathbb{R},\mu)} + \left\|f'\right\|^2_{L_2(\mathbb{R},\frac{1}{\mu})} = \left\|f \circ \mathrm{R}^{-1}\right\|^2_{H^1(\mathbb{T}^d)}$$

$$\|f\|^2_{H^2(\mathbb{R},\mu)} = \|f\|^2_{L_2(\mathbb{R},\mu)} + \left\|f'\right\|^2_{L_2\left(\mathbb{R},\frac{1}{\mu}+\frac{(\mu')^2}{\mu^5}\right)} + \left\|f''\right\|^2_{L_2(\mathbb{R},\frac{1}{\mu^3})} = \left\|f \circ \mathrm{R}^{-1}\right\|^2_{H^2(\mathbb{T})}$$

The normal distribution

density:

$$\mu_{\mathrm{N}}(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-x^2/2}$$



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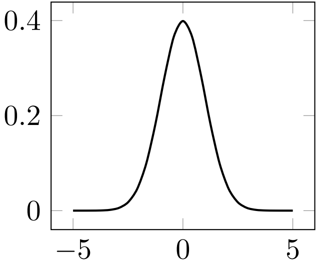

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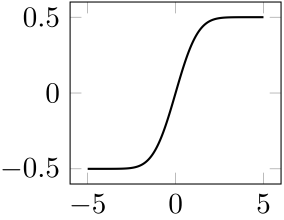

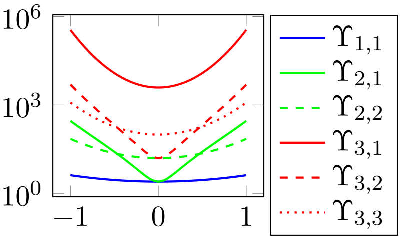

multivariate setting:

$$\|f\|^2_{H^m_{\mathrm{mix}}(\mathbb{R}^d,\mu)} = \sum_{0\le\|\boldsymbol{k}\|_\infty\le m} \left\|\mathrm{D}^{\boldsymbol{k}} f(\boldsymbol{x})\right\|^2_{L_2(\mathbb{R}^d,\Upsilon_{m,\boldsymbol{k}})} \text{ with } \Upsilon_{m,\boldsymbol{k}}(\boldsymbol{x}) := \prod_{i=1}^{d} \Upsilon_{m,k_i}(x_{k_i})$$

further weighted function spaces:

- definition for fractional smoothness via the decay of the Fourier coefficients
- transformation also for Besov regularity possible:
  define norm in $\boldsymbol{B}^s_{2,\infty}(\mathbb{R}^d,\mu)$, such that

$$\left\|f\circ \mathrm{R}^{-1}\right\|_{\boldsymbol{B}^s_{2,\infty}(\mathbb{T}^d)} \lesssim \|f\|_{\boldsymbol{B}^s_{2,\infty}(\mathbb{R}^d,\mu)},$$

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Approximation results on $\mathbb{R}^d$

Theorem ([L., Potts, '22])

Let the density μ_i be in $C^{m-1}(\mathbb{R})$ for $i \in \{1, \dots, d\}$ and let $m \in \mathbb{N}$ be the order of vanishing moments of the wavelet ψ. Let $M \gtrsim rN \log N$ ($r > 1$), $\mathcal{X} \subset \mathbb{R}^d$ be drawn i.i.d at random according to μ, $f \in C(\mathbb{R})$, $\mathcal{Y} = \mathrm{R}(\mathcal{X})$. Then

$$\mathbb{P}\left(\left\| f - (S_n^{\mathcal{Y}}(f \circ \mathrm{R}^{-1})) \circ \mathrm{R} \right\|_{L_2(\mathbb{R}^d,\mu)} \lesssim 2^{-ns} n^{(d-1)/2} \, \|f\|_{\boldsymbol{B}^s_{2,\infty}(\mathbb{R}^d,\mu)} \right) \geq 1 - 2\, M^{-r} \quad \text{if } s < m,$$

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Numerical example

$$\text{RMSE} = \left(\sum_{\boldsymbol{x} \in \mathcal{X}_{\text{test}}} \frac{1}{|\mathcal{X}_{\text{test}}|} |f(\boldsymbol{x}) - \tilde{f}(\boldsymbol{x})|^2 \right)^{1/2}$$

function: $f \colon \mathbb{R}^d \to \mathbb{R}, \quad f(\boldsymbol{x}) = \mathrm{e}^{-\|\boldsymbol{x}\|_2^2}$

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$$\mu_{\mathrm{N}}(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-x^2/2}$$

Numerical example

$$\mathrm{RMSE} = \left(\sum_{\boldsymbol{x} \in \mathcal{X}_{\text{test}}} \frac{1}{|\mathcal{X}_{\text{test}}|} |f(\boldsymbol{x}) - \tilde{f}(\boldsymbol{x})|^2 \right)^{1/2}$$

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- $f \in H^2(\mathbb{R}^d, \mu_{\mathrm{N}}), \quad f \notin H^3(\mathbb{R}, \mu_{\mathrm{N}})$
- $f \in \boldsymbol{B}^{5/2}_{2,\infty}(\mathbb{R}^d, \mu_N)$
- $m = 3 \to m > s$

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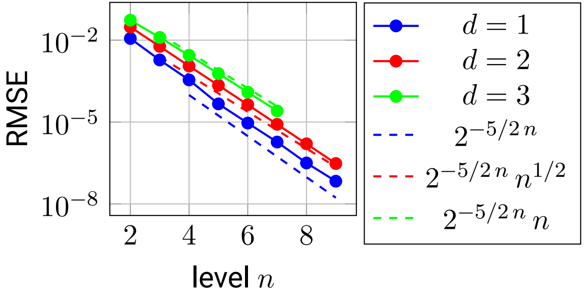

proven error rate:

$$2^{-5/2\,n} n^{(d-1)/2}$$

Numerical example

$$\text{RMSE} = \left(\sum_{\boldsymbol{x} \in \mathcal{X}_{\text{test}}} \frac{1}{|\mathcal{X}_{\text{test}}|} |f(\boldsymbol{x}) - \tilde{f}(\boldsymbol{x})|^2 \right)^{1/2}$$

function: $f \colon \mathbb{R}^d \to \mathbb{R}, \quad f(\boldsymbol{x}) = \mathrm{e}^{-\|\boldsymbol{x}\|_2^2}$
density:

$$\mu_{\mathrm{L}}(x) = \frac{1}{8} \mathrm{e}^{-\frac{|x-2|}{4}}$$

- $f \in H^m(\mathbb{R}^d, \mu_{\mathrm{L}})$ for all $m \in \mathbb{N}$
- $m = 3 \to m = s$

Numerical example

$$\text{RMSE} = \left(\sum_{\boldsymbol{x} \in \mathcal{X}_{\text{test}}} \frac{1}{|\mathcal{X}_{\text{test}}|} |f(\boldsymbol{x}) - \tilde{f}(\boldsymbol{x})|^2 \right)^{1/2}$$

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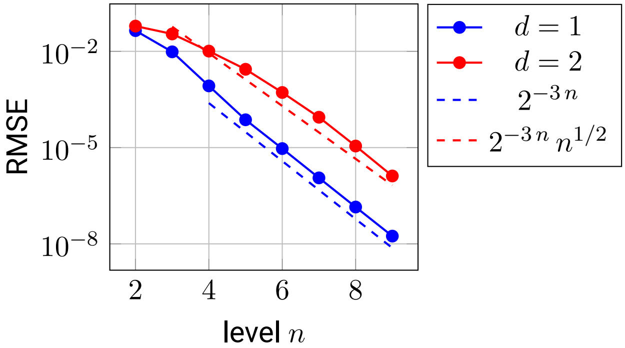


proven error rate:

$$2^{-3n} n^{(d-1)/2}$$

Random Fourier Features

$$f(\boldsymbol{x}) \approx \sum_{j=1}^{N} a_j \mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}_j, \boldsymbol{x} \rangle}$$

- $\boldsymbol{\omega}_j$: draw at random and keep fixed
- a_j: learn from data
- over-parametrized setting $N \gg M$
- background: approximation of a kernel κ by

$$\kappa(\boldsymbol{x}_k, \boldsymbol{x}_\ell) \approx \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}_j, \boldsymbol{x}_k \rangle} \mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}_j, \boldsymbol{x}_\ell \rangle}$$

- different algorithms so far: SRFE, SHRIMP, HARFE, . . .

A. Hashemi, H. Schaeffer, R. Shi, U. Topcu, G. Tran, R. Ward
Generalization Bounds for Sparse Random Feature Expansions
Appl. Comput. Harmon. Anal. 62, 310-330 (2023)

Y. Xie, R. Shi, H. Schaeffer, R. Ward
SHRIMP: Sparser Random Feature Models via Iterative Magnitude Pruning
Proc. Math. Sci, 190, 303–318 (2022)

E. Saha, H. Schaeffer, G. Tran
HARFE: hard-ridge random feature expansion
Sampl. Theory Signal Process. Data Anal. 21, 27 (2023)

A. Rahimi, B. Recht
Random Features for Large-Scale Kernel Machines
Adv. Neural Inf. Process. 20, (2007)

Algorithm

- draw frequencies $(\boldsymbol{\omega}_j)_{j=1}^N \subset \mathbb{R}^d$ according to density $\varrho\colon \mathbb{R}^d \to \mathbb{R}$
- construct random feature matrix $\boldsymbol{A} = \left(\mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}_j, \boldsymbol{x}\rangle}\right)_{j=1,\boldsymbol{x}\in\mathcal{X}}^N$
- $$\boldsymbol{a}^\# = \operatorname*{argmin}_{\boldsymbol{a}} \|\boldsymbol{a}\| \text{ s.t. } \|\boldsymbol{A}\boldsymbol{a} - \boldsymbol{f}\|_2 \le \lambda$$
- optional: prune the index-set $\{1, \ldots, N\}$ iteratively
- construct approximation $f^\#(\boldsymbol{x}) = \sum_{j=1}^N a_j^\# \mathrm{e}^{\mathrm{i}\,\langle \boldsymbol{\omega}_j, \boldsymbol{x}\rangle}$

The distribution ϱ and the smoothness

$$\mathcal{F}(\varrho) := \left\{ f(\boldsymbol{x}) = \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{\omega}) \mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}, \boldsymbol{x} \rangle} \mathrm{d}\boldsymbol{\omega} \mid \|f\|_{\mathcal{F}(\varrho)} := \sup_{\boldsymbol{\omega} \in \mathbb{R}^d} \left| \frac{\hat{f}(\boldsymbol{\omega})}{\varrho(\boldsymbol{\omega})} \right| < \infty \right\}$$

- literature: Gaussian random features: $\varrho_N(\boldsymbol{\omega}) \sim \mathrm{e}^{-\frac{\|\boldsymbol{\omega}\|^2}{2\sigma^2}}$

$\rightarrow$ strong decay condition on the Fourier transform $\hat{f}$

$\rightarrow$ strong smoothness assumption on the function f

idea: using density

$$\varrho_{\Pi}^s \sim \prod_{i \in [d]} \frac{1}{\sigma \left(1 + \omega_i^2 / \sigma^2\right)^s}$$

work in progress:

$$H_{\text{mix}}^r(\mathbb{R}^d) \subseteq \mathcal{F}(\varrho_{\Pi}^s) \text{ if } s > \tfrac{1}{2}, r < 2s - \tfrac{1}{2},$$

$$\lim_{r \to 2s - 1/2} H_{\text{mix}}^r(\mathbb{R}^d) = \mathcal{F}(\varrho_{\Pi}^s).$$

In the literature so far:

- finite second moment of feature density ϱ is needed $\to$ can be relaxed

Work in progess:

- Matrix $\boldsymbol{A} = \left(\mathrm{e}^{\mathrm{i}\langle \boldsymbol{\omega}, \boldsymbol{x}\rangle}\right)_{j=1, \boldsymbol{x}\in\mathcal{X}}^{N}$ is well-conditioned w.h.p. if
  - $N \geq 2M$
  - $\sigma\gamma\sqrt{d} \gtrsim \log M$ $\qquad (\gamma, \sigma :$ scaling parameters of $\mu, \varrho)$
  - μ fulfills small ball property: $\mathbb{P}(\|\boldsymbol{x} - \boldsymbol{x}'\| > \delta) > \varepsilon$
  - $|\hat{\varrho}(\boldsymbol{x})| \lesssim \mathrm{e}^{-\|\boldsymbol{x}\|_2}$

The interpolation case

$$\boldsymbol{a}^{\#} = \arg \min_{\boldsymbol{f}=\boldsymbol{A}\boldsymbol{a}} \|\boldsymbol{a}\|_2 = \boldsymbol{A}^*(\boldsymbol{A}\boldsymbol{A}^*)^{-1}\boldsymbol{f}, \quad N \geq \frac{4}{\epsilon^2}\left(1 + \sqrt{\frac{1}{2}\log\left(\frac{1}{\delta}\right)}\right)^2,$$

$$\mathbb{P}\left(\left\|f - f^{\#}\right\|_{L_2(\mathbb{R}^d,\mu)} \lesssim \left(1 + \log\left(\frac{1}{\delta}\right)\right)^{1/4} M^{1/4}\right) \epsilon \|f\|_{\mathcal{F}(\varrho)}\Bigg) \geq 1 - \delta$$

Low-dimensional structures in high-dimensions

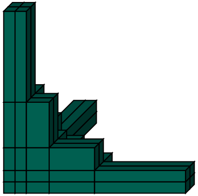
ANOVA (Analysis of variance) decomposition :

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{u} \subseteq \{1,\ldots,d\}} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}})$$

properties:

- $f_\varnothing = \int_{\mathbb{R}} f(\boldsymbol{x})\mu(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$
- $\int_{\mathbb{R}} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}})\mu(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = 0, \quad \boldsymbol{u} \neq \boldsymbol{v}$

truncation: $f(\boldsymbol{x}) \approx \sum_{|\boldsymbol{u}| \leq q} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}})$



hyperbolic index-set I_3

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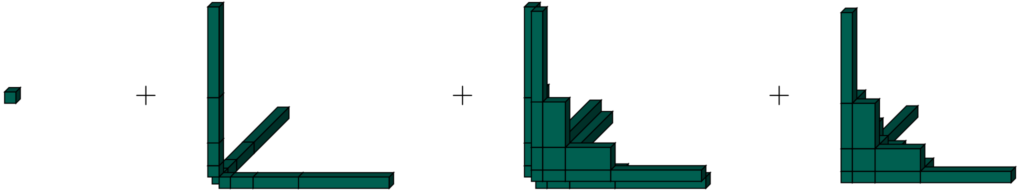

$$I_3^{\varnothing} \quad \cup \quad I_3^{\{1\}} \cup I_3^{\{2\}} \cup I_3^{\{3\}} \quad \cup \quad I_3^{\{1,2\}} \cup I_3^{\{1,3\}} \cup I_3^{\{2,3\}} \quad \cup \quad I_3^{\{1,2,3\}}$$

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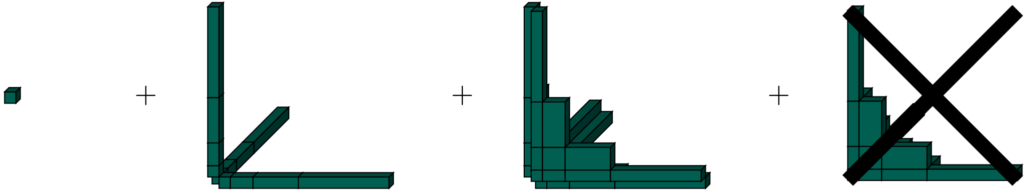

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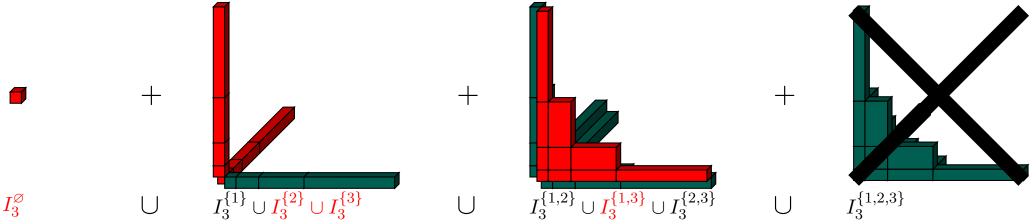


ANOVAapprox

$$f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) \approx \sum_{(\boldsymbol{j},\boldsymbol{k})\in I^{\boldsymbol{u}}} a_{\boldsymbol{j},\boldsymbol{k}} \psi^{\mathrm{per}}_{\boldsymbol{j},\boldsymbol{k}}(\mathrm{R}_{\boldsymbol{u}}^{-1}(\boldsymbol{x}_{\boldsymbol{u}}))$$

$\rightarrow$ choosing index-set with $|\operatorname{supp} \boldsymbol{j}| \leq q$

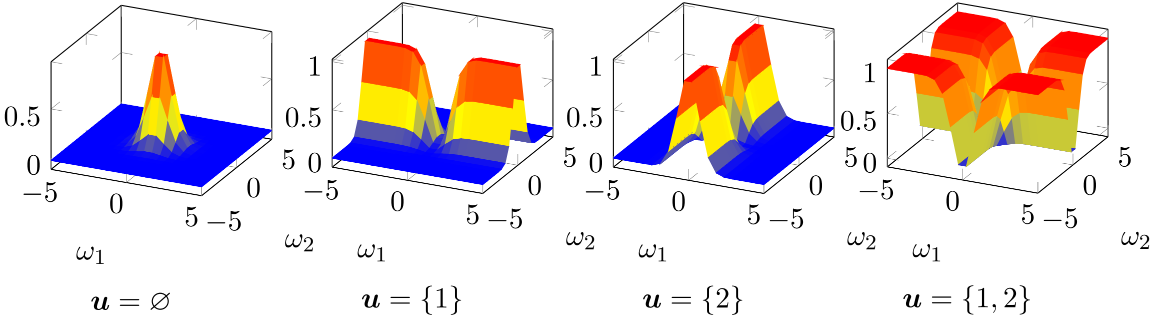
- approximate variances $\sigma^2(f_{\boldsymbol{u}})$ by $\sigma^2((S_n^{\mathcal{Y}}(f \circ \mathrm{R}^{-1}))_{\boldsymbol{u}})$ from coefficients $a_{\boldsymbol{j},\boldsymbol{k}}$
- second approximation: using only important ANOVA terms, increase accuracy for important ANOVA terms

M. Schmischke, L. Lippert, F.Nestler
NFFT/ANOVAapprox.jl: v1.1.7 (v1.1.7)
Zenodo. https://doi.org/10.5281/zenodo.7070795

L. Lippert, D. Krumm, D. Potts, S. Odenwald
Estimating vertical ground reaction forces from plantar pressure using interpretable high-dimensional approximation
submitted to Sports Eng.

Sparse Random Fourier Features

- similar idea: draw q-sparse frequencies random:
  For each $\boldsymbol{u} \subset \{1, \dots, d\}$ with $|\boldsymbol{u}| = q$ draw random $\boldsymbol{\omega}_{\boldsymbol{u}}$ and $\boldsymbol{\omega}_{\boldsymbol{u}^c} = \mathbf{0}$
- $\mathrm{e}^{\langle \boldsymbol{\omega}_j, \cdot \rangle}$ is no orthonormal system
- $f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{\omega}) E(\boldsymbol{x}, \boldsymbol{\omega}, \mu, \boldsymbol{u}) \mathrm{d}\boldsymbol{\omega}$



Trafo approach

- fast multiplication with matrix $\boldsymbol{A}$ available $\to$ fast algorithm for big number of samples M
- direct connection between ANOVA terms and coefficients $a_{\boldsymbol{j},\boldsymbol{k}}$
- function spaces $H^s_{\mathrm{mix}}(\mathbb{R}^d, \mu)$

$\to$ approximation rates are transferred from $\mathbb{T}^d$ to $\mathbb{R}^d$

Random Fourier Features

- no fast algorithm available, but more parameters possible for low number of samples M (compared to dimension d)
- can be interpreted as a neural network with two layers
- function spaces $\mathcal{F}(\varrho)$
- theoretical error estimates possible, with complicated assumptions
- sensitive to the parameter choice

Thank you for your attention