Learning Anisotropy for ANOVA Approximation

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Rhein-Ruhr-Workshop

09.02.2024

UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Let $f\colon \mathbb{T}^d \to \mathbb{C},\ \mathbf{x} \mapsto f(\mathbf{x})$ be a function in $C(\mathbb{T}^d)$.

Task

Given: $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_M\} \subset \mathbb{T}^d$ and $\mathbf{y} \in \mathbb{C}^M$ with $f(\mathbf{x}_j) = y_j$, $j = 1, \dots, M$
Goal: find approximation $\tilde{f}(\mathbf{x}) \approx f(\mathbf{x})$.

Ansatz: Use Fourier series

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} c_{\mathbf{k}}(f) \exp\left(2\pi\mathrm{i}\left\langle \mathbf{k}, \mathbf{x}\right\rangle\right), \ \mathbf{x} \in \mathbb{T}^d$$

with the Fourier coefficients $c_{\mathbf{k}}(f) := \left\langle f, \exp\left(2\pi\mathrm{i}\left\langle \mathbf{k}, \cdot\right\rangle\right)\right\rangle_{\mathrm{L}_2}$.

Set $\tilde{f}(\mathbf{x}) := \sum_{\mathbf{k} \in \mathcal{I}} \hat{f}_{\mathbf{k}} \exp\left(2\pi\mathrm{i}\left\langle \mathbf{k}, \mathbf{x}\right\rangle\right)$ and find $\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f) \in \mathbb{C}$.
We have to choose the index set $\mathcal{I} \subset \mathbb{Z}^d$. We call $|\mathcal{I}| = B$ frequency budget.

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Least squares approximation

We get $\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f) \in \mathbb{C}$, $\mathbf{k} \in \mathcal{I}$ through

$$\left\| \left(\tilde{f}(\mathbf{x}_j) - f(\mathbf{x}_j)\right)_{j=1}^{d} \right\|_2^2 = \left\| \underbrace{\begin{pmatrix} \phi_{\mathbf{k}_1}(\mathbf{x}_1) & \cdots & \phi_{\mathbf{k}_B}(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_{\mathbf{k}_1}(\mathbf{x}_M) & \cdots & \phi_{\mathbf{k}_B}(\mathbf{x}_M) \end{pmatrix}}_{=:\mathbf{A} \in \mathbb{C}^{M \times B},\ M \geq B} \underbrace{\begin{pmatrix} \hat{f}_{\mathbf{k}_1} \\ \vdots \\ \hat{f}_{\mathbf{k}_B} \end{pmatrix}}_{\in \mathbb{C}^B} - \underbrace{\begin{pmatrix} y_1 \\ \vdots \\ y_M \end{pmatrix}}_{\in \mathbb{C}^M} \right\|_2^2 \longrightarrow \min$$

with $\phi_{\mathbf{k}}(\mathbf{x}) = \exp\left(2\pi \mathrm{i} \langle \mathbf{k}, \mathbf{x} \rangle\right)$

and $\mathcal{I} = \{\mathbf{k}_1, \ldots, \mathbf{k}_B\} \subset \mathbb{Z}^d$.

The solution is given by $(\hat{f}_{\mathbf{k}})_{\mathbf{k} \in \mathcal{I}} = (\mathbf{A}^* \mathbf{A})^{-1} \mathbf{A}^* \mathbf{y}$.

This can be computed efficiently using a least squares solver, together with NFFT if $\mathcal{I}$ is a box.
It is theoretically shown that $B \sim M / \log(M)$ implies that $\mathbf{A}$ has a good condition number with high probability.[1]

[1] L. Kämmerer, T. Ullrich, T. Volkmer, **Worst-case recovery guarantees for least squares approximation using random samples**, Constr. Approx., 54:295–352, (2021).

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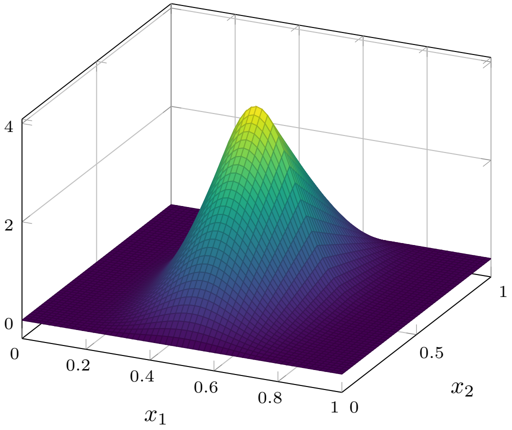
Example

$$f(x_1, x_2) = b_6(x_1)b_2(x_2)$$



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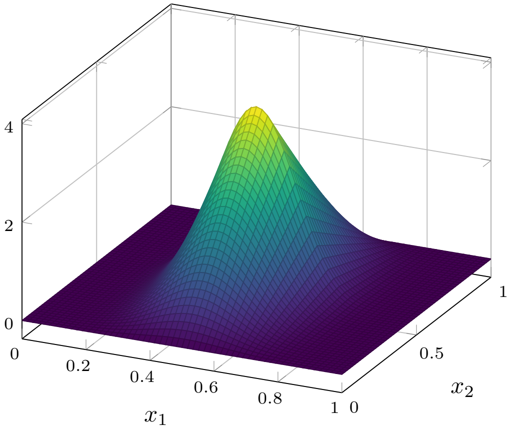
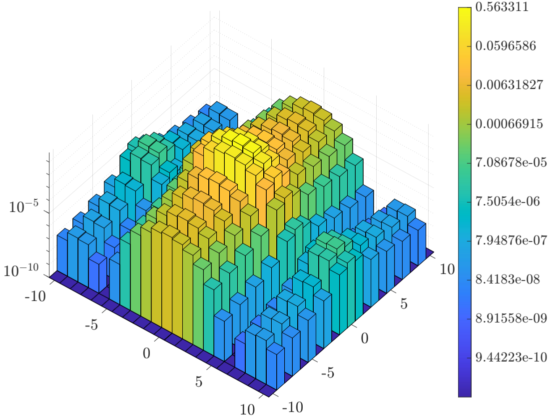


$\hat{f}_{\mathbf{k}}$ for $\mathbf{k} \in \mathcal{I} = \{-10, \ldots, 10\}^2$,
$|B| = B = 441$



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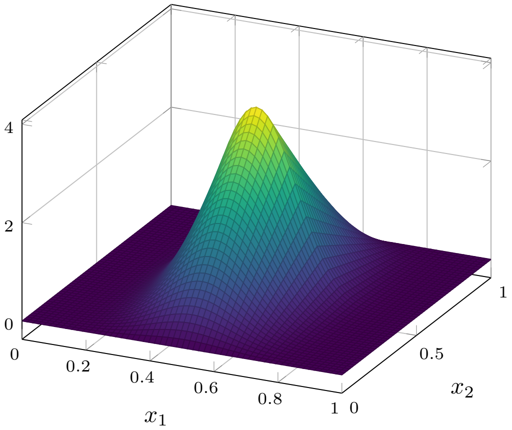

$\hat{f}_{\mathbf{k}}$ for $\mathbf{k} \in \mathcal{I} = \{-4, \ldots, 4\} \times \{-24, \ldots, 24\}$,
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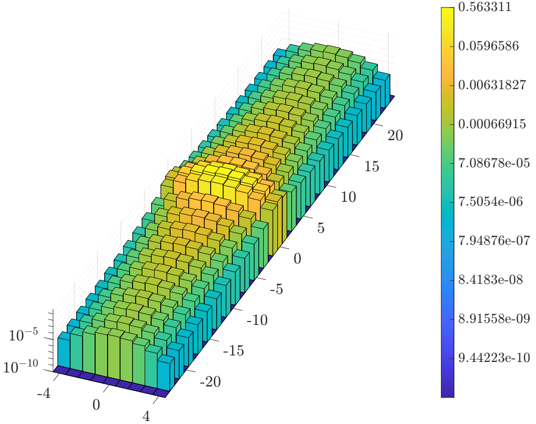

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For the projection $P_{\mathcal{I}} f := \underset{g \in \operatorname{span}\{\exp(2\pi \mathrm{i} \langle \mathbf{k}, \cdot \rangle)\}_{\mathbf{k} \in \mathcal{I}}}{\arg\min} \|g - f\|_{L_2}^2$ we get the projection error

$$\|f - P_{\mathcal{I}} f\|_{\mathrm{L}_2}^2 = \|\sum_{\mathbf{k} \notin \mathcal{I}} c_{\mathbf{k}}(f) \exp\left(2\pi \mathrm{i} \langle \mathbf{k}, \cdot \rangle\right)\|_{\mathrm{L}_2}^2 = \sum_{\mathbf{k} \notin \mathcal{I}} |c_{\mathbf{k}}(f)|^2$$

We get the following for the function $f(x_1, x_2) = b_6(x_1) b_2(x_2)$:

frequency square $\mathcal{I}$:

$$\mathcal{I} = \{-10, -9, \dots, 10\}^2$$
$$|\mathcal{I}| = B = 441$$
$$\|f - P_{\mathcal{I}} f\|_{\mathrm{L}_2}^2 \approx 4.027 \cdot 10^{-5}$$

optimal frequency box $\mathcal{I}^*$:

$$\mathcal{I}^* = \{-4, -3, \dots, 4\} \times \{-24, -23, \dots, 24\}$$
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Outline

We define anisotropic Sobolev spaces[2]

$$H^{s_1,\dots,s_d} := \left\{ f \in L_2 \,\middle|\, D^{\boldsymbol{\alpha}} f \in L_2 \text{ for } \boldsymbol{\alpha} = (\alpha_1,\dots,\alpha_d) \in \mathbb{N}_0^d \text{ with } \frac{\alpha_1}{s_1} + \dots + \frac{\alpha_d}{s_d} \le 1 \right\}$$

with the norm $\|f\|^2_{H^{s_1,\dots,s_d}} := \sum_{\mathbf{k}\in\mathbb{Z}^d} |\max\{1, k_1^{s_1},\dots,k_d^{s_d}\}\hat{c}_{\mathbf{k}}(f)|^2$.

Lemma

Let $\mathbf{N} = (N_1,\dots,N_d) \in (2\mathbb{N}_0)^d$. *When projecting functions* f *from anisotropic Sobolev spaces* $H^{s_1,\dots,s_d}$ *to frequency boxes*

$$\mathcal{I}_{\mathbf{N}} := \bigtimes_{j=1}^{d} \begin{cases} \{0\} & \text{if } N_j = 0 \\ [-N_j/2, N_j/2) \cap \mathbb{Z} & \text{otherwise,} \end{cases}$$

we obtain

$$\sup_{\|f\|_{H^{s_1,\dots,s_d}} \le 1} \|f - P_{\mathcal{I}_{\mathbf{N}}} f\|^2_{L_2} = \left(\max\left\{1, \left(\frac{N_1}{2}\right)^{s_1}, \dots, \left(\frac{N_d}{2}\right)^{s_d} \right\}\right)^{-2}.$$

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frequency cubes $\mathcal{I}_{\mathbf{N}}$

with $N_j = \sqrt[d]{B}$

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Example

$d = 2,\ s_1 = 1,\ s_2 = 10$

$$\sup_{\|f\|_{H^{1,10}} \le 1} \|f - P_{\mathcal{I}_{\mathbf{N}}} f\|_{L_2}^2 \sim B^{-1} \qquad \sup_{\|f\|_{H^{1,10}} \le 1} \|f - P_{\mathcal{I}_{\mathbf{N}^*}} f\|_{L_2}^2 \sim B^{-\frac{20}{11}}$$

Example

$f(x_1, x_2) = b_6(x_1) b_2(x_2)$ has the smoothness $s_1 = \frac{11}{2}$ and $s_2 = \frac{3}{2}$

$$\|f - P_{\mathcal{I}_{\mathbf{N}}} f\|_{L_2}^2 \lesssim B^{-\frac{3}{2}} \qquad \|f - P_{\mathcal{I}_{\mathbf{N}^*}} f\|_{L_2}^2 \lesssim B^{-\frac{33}{14}} \lesssim B^{-2.357}$$

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How to find the smoothness $s_1, \dots, s_d$?

Example: $d = 2$, find smoothness s_1

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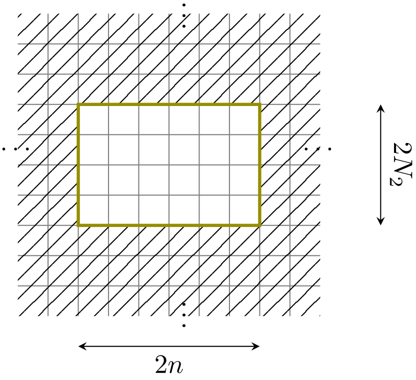
$$\mathcal{I}_{\tilde{\mathbf{N}}(n)} = \{-n, \dots, n-1\} \times \{-N_2, \dots, N_2 - 1\}$$

$$\left\| f - P_{\mathcal{I}_{\tilde{\mathbf{N}}(n)}} f \right\|_{\mathrm{L}_2}^2 = \Big\| \sum_{\mathbf{k} \notin \mathcal{I}_{\tilde{\mathbf{N}}(n)}} c_{\mathbf{k}}(f) \Big\|_{\mathrm{L}_2}^2 = \sum_{\mathbf{k} \notin \mathcal{I}_{\tilde{\mathbf{N}}(n)}} |c_{\mathbf{k}}(f)|^2 = \sum_{\substack{k_1 \in \mathbb{Z} \\ |k_2| > N_2}} |c_{\mathbf{k}}(f)|^2 + \sum_{\substack{|k_1| > n \\ |k_2| \le N_2}} |c_{\mathbf{k}}(f)|^2 \lesssim A + C_j n^{-2s_j}$$



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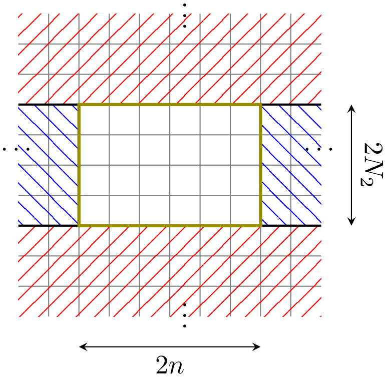

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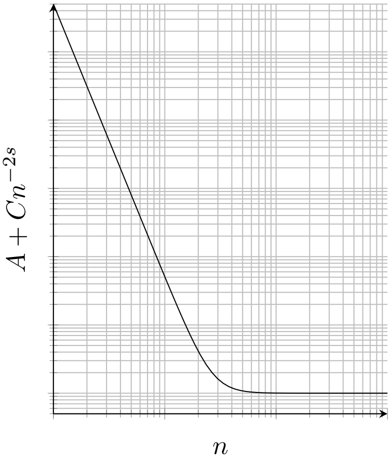
\left\| f - P_{\mathcal{I}_{\tilde{\mathbf{N}}(n)}} f \right\|_{\mathrm{L}_2}^2 &= \Big\| \sum_{\mathbf{k} \notin \mathcal{I}_{\tilde{\mathbf{N}}(n)}} c_{\mathbf{k}}(f) \Big\|_{\mathrm{L}_2}^2 \\
&= \sum_{\mathbf{k} \notin \mathcal{I}_{\tilde{\mathbf{N}}(n)}} |c_{\mathbf{k}}(f)|^2 \\
&= \sum_{\substack{k_1 \in \mathbb{Z} \\ |k_2| > N_2}} |c_{\mathbf{k}}(f)|^2 + \sum_{\substack{|k_1| > n \\ |k_2| \le N_2}} |c_{\mathbf{k}}(f)|^2 \\
&\lesssim A + C_j n^{-2 s_j}
\end{aligned}$$



Lemma

Let $f\colon \mathbb{T}^d \to \mathbb{C}$ *be a function and* $\tilde{f} = \sum_{\mathbf{k}\in\mathcal{I}} \hat{f}_k \exp(2\pi\mathrm{i}\langle \mathbf{k},\cdot\rangle)$ *an approximation. Then*

$$\frac{1}{2}\sum_{\mathbf{k}\notin\mathcal{I}} |\hat{f}_{\mathbf{k}}|^2 - \|f-\tilde{f}\|_{\mathrm{L}_2}^2 \le \|f - P_{\mathcal{I}} f\|_{\mathrm{L}_2}^2 \le 2\sum_{\mathbf{k}\notin\mathcal{I}} |\hat{f}_{\mathbf{k}}|^2 + \|f-\tilde{f}\|_{\mathrm{L}_2}^2 .$$

It follows $\sum_{\mathbf{k}\notin\mathcal{I}_{\tilde{\mathbf{N}}(n)}} |\hat{f}_{\mathbf{k}}|^2 \sim \|f - P_{\mathcal{I}_{\tilde{\mathbf{N}}(n)}} f\|_{\mathrm{L}_2}^2 \lesssim A + C_j n^{-2s_j}$ if $\|f-\tilde{f}\|_{\mathrm{L}_2}^2$ is small.

Lemma

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$$\frac{1}{2}\sum_{\mathbf{k}\notin\mathcal{I}} |\hat{f}_{\mathbf{k}}|^2 - \|f - \tilde{f}\|_{\mathrm{L}_2}^2 \le \|f - P_{\mathcal{I}} f\|_{\mathrm{L}_2}^2 \le 2\sum_{\mathbf{k}\notin\mathcal{I}} |\hat{f}_{\mathbf{k}}|^2 + \|f - \tilde{f}\|_{\mathrm{L}_2}^2 .$$

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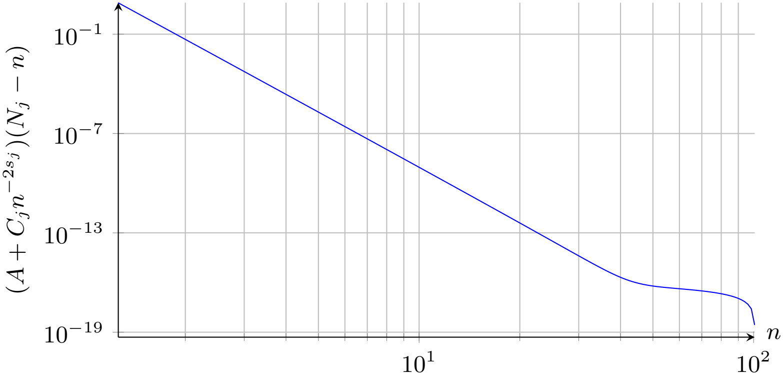
How to find the smoothness s_j numerically from given $\hat{f}_{\mathbf{k}}$ for $\mathbf{k} \in \mathcal{I}_{\mathbf{N}}$?

$$\sum_{\mathbf{k} \notin \mathcal{I}_{\tilde{\mathbf{N}}(n)}} |\hat{f}_{\mathbf{k}}|^2 \approx \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}} \setminus \mathcal{I}_{\tilde{\mathbf{N}}(n)}} |\hat{f}_{\mathbf{k}}|^2 \lesssim (A + C_j n^{-2s_j})(N_j - n)$$



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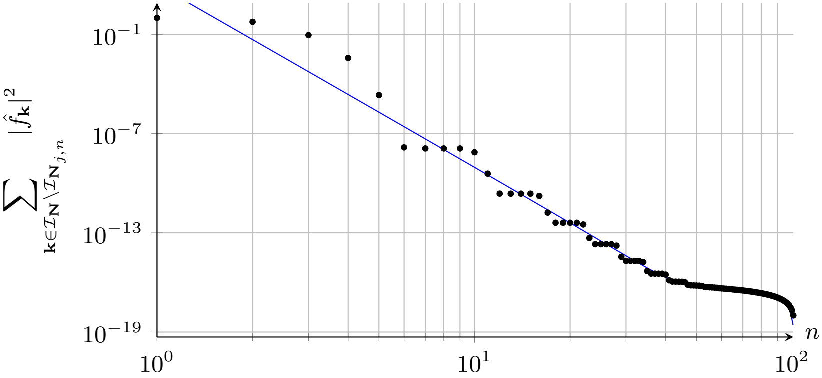

$$f(x_1, x_2) = b_6(x_1) b_2(x_2)$$

$h(n) = Dn^{-2t}$

$t =$

$D_u \approx$

$D_l \approx$

Hull width $\frac{D_u}{D_l} \approx$

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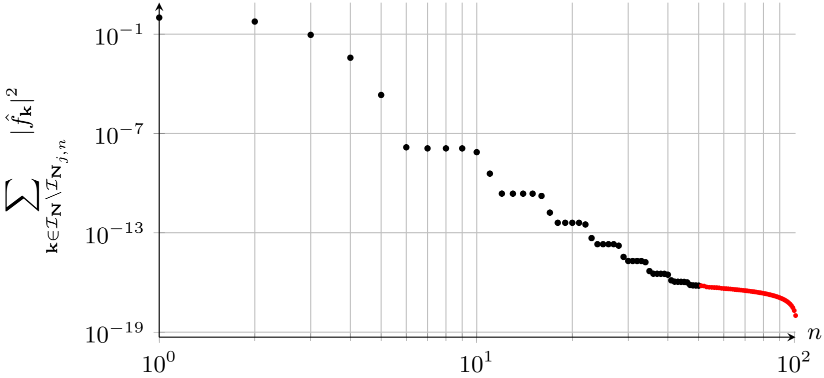

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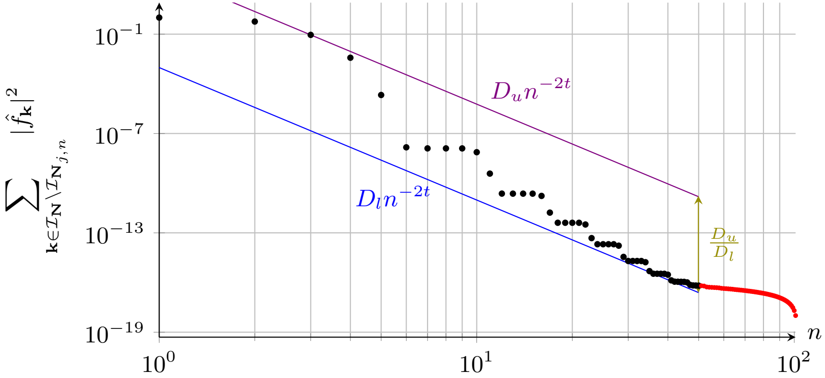

$$f(x_1, x_2) = b_6(x_1) b_2(x_2)$$

$$h(n) = D n^{-2t}$$

$$t = 4$$

$$D_u \approx 592.8867$$

$$D_l \approx 0.000958$$

Hull width $\frac{D_u}{D_l} \approx 618879$

How to find the smoothness s_j numerically from given $\hat{f}_{\mathbf{k}}$ for $\mathbf{k} \in \mathcal{I}_{\mathbf{N}}$?

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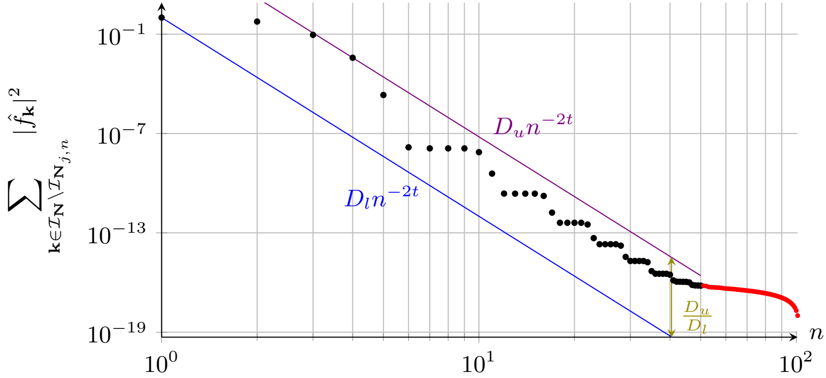

$$f(x_1, x_2) = b_6(x_1) b_2(x_2)$$

$$h(n) = D n^{-2t}$$

$$t = 6$$

$$D_u \approx 63268.7$$

$$D_l \approx 1$$

Hull width $\frac{D_u}{D_l} \approx 63268$

How to find the smoothness s_j numerically from given $\hat{f}_{\mathbf{k}}$ for $\mathbf{k} \in \mathcal{I}_{\mathbf{N}}$?

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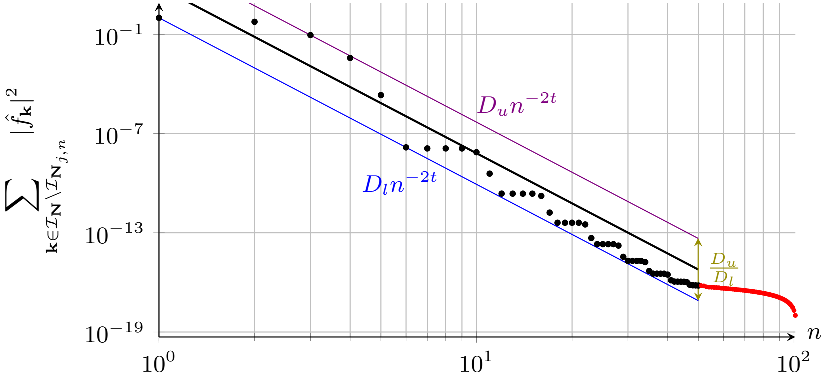


$$f(x_1, x_2) = b_6(x_1) b_2(x_2)$$

$$h(n) = Dn^{-2t}$$

$$t = 5$$

$$D_u \approx 5754.04$$

$$D_l \approx 1$$

Hull width $\frac{D_u}{D_l} \approx 5754$

Theorem (Bartel, S. '24)

Let $f : \mathbb{T}^d \to \mathbb{C}$ *be a function with* $C_l n^{-2s} \leq \|f - P_{\mathcal{I}_{\tilde{\mathbf{N}}(n)}}\| \leq C_u n^{-2s}$, $C_l, C_u, s > 0,\ n \in \mathbb{N}$ *and* $\tilde{f} = \sum_{\mathbf{k}\in\mathcal{I}_\mathbf{N}} \hat{f}_k \exp(2\pi\mathrm{i}\,\langle \mathbf{k}, \cdot\rangle)$ *an approximation. Let further* $M \in \mathbb{N}$ *and approximate* s *by*

$$t := \operatorname*{arg\,min}_{r\in\mathbb{R}} \left(\frac{\max_{m\in[M]} (m^{2r} \sum_{\mathbf{k}\notin\mathcal{I}_{\tilde{\mathbf{N}}(n)}} |\hat{f}_\mathbf{k}|^2)}{\min_{m\in[M]} (m^{2r} \sum_{\mathbf{k}\notin\mathcal{I}_{\tilde{\mathbf{N}}(n)}} |\hat{f}_\mathbf{k}|^2)} \right) \left[\begin{matrix} \} =: D_u \\ \} =: D_l \end{matrix} \right].$$

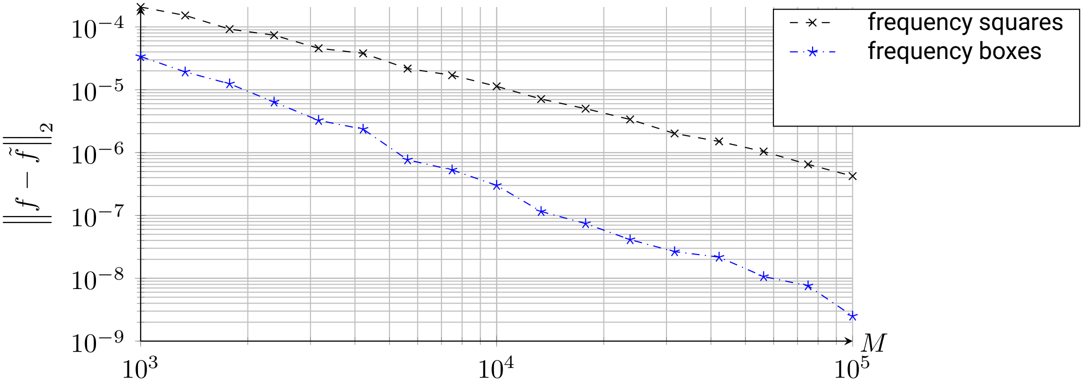
Then

$$|t - s| \leq \frac{\log(\delta)}{\log(M)} \quad \textit{and} \quad (1/2 - \gamma)\sqrt{\delta}^{-1} C_l \leq \sqrt{D_u D_l} \leq (2 + 2\gamma)\sqrt{\delta} C_u$$

holds with $\gamma := \|f - \tilde{f}\|^2_{\mathrm{L}_2} / \|f - P_{\mathcal{I}_{\tilde{\mathbf{N}}(n)}}\|^2_{\mathrm{L}_2}$ *and* $\delta := \frac{4+4\gamma}{1-2\gamma} \frac{C_u}{C_l}$.

Numerical example

$$f(x_1, x_2) = b_6(x_1)b_2(x_2)$$



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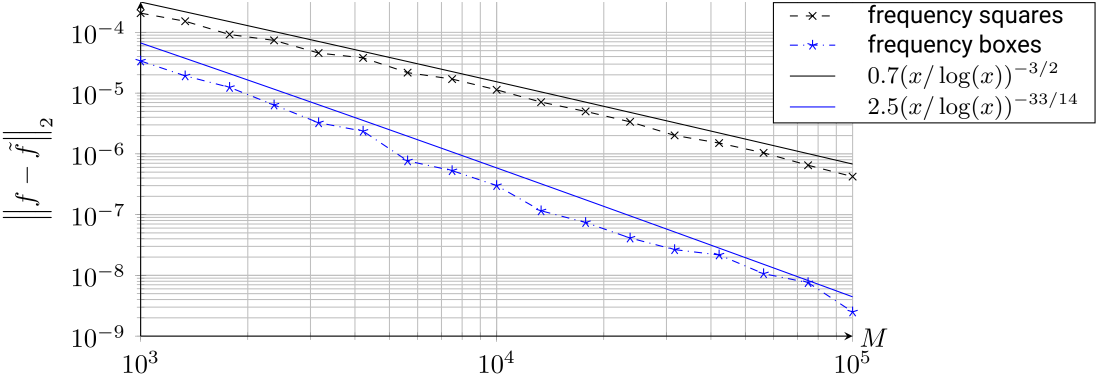

Problem: curse of dimensionality, evaluation of trigonometric polynomials $\sum_{\mathbf{k}\in\mathcal{I}} \hat{f}_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{x}_j)$ at M points performed with NFFT has the computational cost $\mathcal{O}(|\mathcal{I}|\log|\mathcal{I}| + |\log\epsilon|^d M)$

Theorem: Decomposition in ANOVA terms[3]

$$f = f_\emptyset \qquad \ldots 1 \times \text{ constant function}$$
$$+ f_{\{1\}} + f_{\{2\}} + \ldots + f_{\{d\}} \qquad \ldots d \times \text{ univariate functions}$$
$$+ f_{\{1,2\}} + f_{\{1,3\}} + \ldots + f_{\{d-1,d\}} \qquad \ldots \binom{d}{2} \times \text{ bivariate functions}$$
$$+ f_{\{1,2,3\}} + f_{\{1,2,4\}} + \ldots + f_{\{d-2,d-1,d\}} \qquad \ldots \binom{d}{3} \times \text{ trivariate funktions}$$
$$+ f_{\{1,2,3,4\}} + f_{\{1,2,3,5\}} + \ldots + f_{\{d-3,d-2,d-1,d\}}$$
$$\vdots$$
$$+ f_{\{1,2,\ldots,d\}} \qquad \ldots 1 \times d\text{-variate function}$$

[3] Kuo, F. Y. and Sloan, I. H. and Wasilkowski, G. W. and Woźniakowski, H., **On decompositions of multivariate functions**, Math. Comput., (2010).

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[3] Kuo, F. Y. and Sloan, I. H. and Wasilkowski, G. W. and Woźniakowski, H., **On decompositions of multivariate functions**, Math. Comput., (2010).

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Theorem: Decomposition in ANOVA terms

$$f \approx f_{\emptyset} \qquad \ldots 1 \times \text{ constant function}$$
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④ Schmischke, M., **Interpretable Approximation of High-Dimensional Data based on the ANOVA Decomposition**, Thesis, Universitätsverlag Chemnitz, (2022).

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Theorem: Decomposition in ANOVA terms approximated by trigonometric polynomials

$$
\begin{aligned}
f \approx\ & f_{\emptyset} && \dots 1 \times \text{ constant function} \\
& + f_{\{1\}}^{N_{\{1\},1}} + f_{\{2\}}^{N_{\{2\},2}} + \dots + f_{\{d\}}^{N_{\{d\},d}} && \dots d \times \text{ univariate functions} \\
& + f_{\{1,2\}}^{N_{\{1,2\},1}, N_{\{1,2\},2}} + f_{\{1,3\}} + \dots + f_{\{d-1,d\}}^{N_{\{d-1,d\},d-1}, N_{\{d-1,d\},d}} && \dots \binom{d}{2} \times \text{ bivariate functions} \\
& + f_{\{1,2,3\}} + f_{\{1,2,4\}}^{N_{\{1,2,4\},1}, N_{\{1,2,4\},2}, N_{\{1,2,4\},4}} + \dots + f_{\{d-2,d-1,d\}} && \dots \binom{d}{3} \times \text{ trivariate funktions} \\
& + f_{\{1,2,3,4\}} + f_{\{1,2,3,5\}} + \dots + f_{\{d-3,d-2,d-1,d\}} \quad ④ \\
& \vdots \\
& + f_{\{1,2,\dots,d\}} \quad ④
\end{aligned}
$$

$f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^d} c_{\mathbf{k}}(f) \exp\left(2\pi\mathrm{i}\langle\mathbf{k},\mathbf{x}\rangle\right)$

ANOVA terms

An ANOVA term is defined as

$$f_{\mathbf{u}}\colon \mathbb{T}^d \to \mathbb{C},\ f_{\mathbf{u}}(\mathbf{x}) := \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f) \underbrace{\exp\left(2\pi\mathrm{i}\langle\mathbf{k},\mathbf{x}\rangle\right)}_{=:\phi_{\mathbf{k}}(\mathbf{x})}, \quad f_{\mathbf{u}} \in H^{s_{u_1},\dots s_{u_{|\mathbf{u}|}}}$$

for a subset of indices $\mathbf{u} \subset \{1,\dots,d\}$.

$$f = \sum_{\mathbf{u}\in\mathcal{P}([d])} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}}$$

$$f_{\mathbf{u}} = \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} = \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} \approx \sum_{\mathbf{k}\in\tilde{\mathcal{I}}_{\mathbf{N}_{\mathbf{u}}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} \approx \sum_{\mathbf{k}\in\tilde{\mathcal{I}}_{\mathbf{N}_{\mathbf{u}}}} \hat{f}_{\mathbf{k}}\phi_{\mathbf{k}}$$

$$\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f)$$

$f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^d} c_{\mathbf{k}}(f) \exp\left(2\pi \mathrm{i} \langle \mathbf{k}, \mathbf{x}\rangle\right)$

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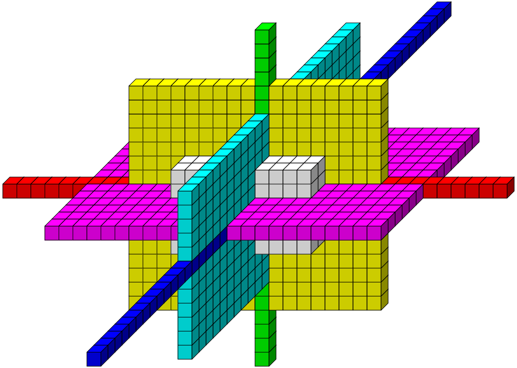
$$\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f)$$

$$\tilde{\mathcal{I}}_{\mathbf{N_u}} := \bigtimes_{j=1}^{d} \begin{cases} \{0\}, & \text{if } N_j = 0 \\ [-N_{\mathbf{u},j}/2, N_{\mathbf{u},j}/2) \cap \mathbb{Z} \setminus \{0\}, & \text{otherwise} \end{cases}, \qquad \mathcal{I}_{\mathbf{N}} = \bigcup_{\mathbf{u} \in U} \tilde{\mathcal{I}}_{\mathbf{N_u}}$$



$\tilde{\mathcal{I}}_{\mathbf{N}_{\{1\}}}$ with $\mathbf{N}_{\{1\}} = \begin{pmatrix} 18 & 0 & 0 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{2\}}}$ with $\mathbf{N}_{\{2\}} = \begin{pmatrix} 0 & 25 & 0 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{3\}}}$ with $\mathbf{N}_{\{3\}} = \begin{pmatrix} 0 & 0 & 12 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{1,2\}}}$ with $\mathbf{N}_{\{1,2\}} = \begin{pmatrix} 12 & 7 & 0 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{1,3\}}}$ with $\mathbf{N}_{\{1,3\}} = \begin{pmatrix} 9 & 0 & 8 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{2,3\}}}$ with $\mathbf{N}_{\{2,3\}} = \begin{pmatrix} 0 & 12 & 6 \end{pmatrix}^\top$

$\tilde{\mathcal{I}}_{\mathbf{N}_{\{1,2,3\}}}$ with $\mathbf{N}_{\{1,2,3\}} = \begin{pmatrix} 5 & 3 & 3 \end{pmatrix}^\top$

$$f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^d} c_{\mathbf{k}}(f) \exp(2\pi\mathrm{i}\langle\mathbf{k},\mathbf{x}\rangle)$$

ANOVA terms

An ANOVA term is defined as

$$f_{\mathbf{u}}\colon \mathbb{T}^d \to \mathbb{C},\ f_{\mathbf{u}}(\mathbf{x}) := \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f) \underbrace{\exp(2\pi\mathrm{i}\langle\mathbf{k},\mathbf{x}\rangle)}_{=:\phi_{\mathbf{k}}(\mathbf{x})}, \quad f_{\mathbf{u}} \in H^{s_{u_1},\dots s_{u_{|\mathbf{u}|}}}$$

for a subset of indices $\mathbf{u} \subset \{1,\dots,d\}$.

$$f = \sum_{\mathbf{u}\in\mathcal{P}([d])} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}} \qquad f \approx \sum_{\mathbf{u}\in U} f_{\mathbf{u}}$$

$$f_{\mathbf{u}} = \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} = \sum_{\substack{\mathbf{k}\in\mathbb{Z}^d \\ \operatorname{supp}\mathbf{k}=\mathbf{u}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} \approx \sum_{\mathbf{k}\in\tilde{\mathcal{I}}_{\mathbf{N}_{\mathbf{u}}}} c_{\mathbf{k}}(f)\phi_{\mathbf{k}} \rightsquigarrow f_{\mathbf{u}} \approx \sum_{\mathbf{k}\in\tilde{\mathcal{I}}_{\mathbf{N}_{\mathbf{u}}}} \hat{f}_{\mathbf{k}}\phi_{\mathbf{k}}$$

$$\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f)$$

Theorem (Bartel, S. '24)

Let $B \in \mathbb{N}$ be a frequency budget and $U \subseteq \mathcal{P}(\{1,\dots,d\})$. Further, let $C_{\mathbf{u},j} > 0$ and $s_{\mathbf{u},j} > 0$ already computed, $j \in \mathbf{u}$ for $\mathbf{u} \in U$. Then the solution of

$$\begin{aligned}\min_{\mathbf{N}} \; & \|f - P_{\mathcal{I}_\mathbf{N}} f\|_{L_2}^2 \\ \text{s.t.} \; & |\mathcal{I}_\mathbf{N}| = B\end{aligned} \quad \iff \quad \begin{aligned}\min_{\mathbf{N}} \; & \sum_{\mathbf{u}\in U} \sum_{j\in\mathbf{u}} C_{\mathbf{u},j} N_{\mathbf{u},j}^{-2s_{\mathbf{u},j}} \\ \text{s.t.} \; & \sum_{\mathbf{u}\in U} \prod_{j\in\mathbf{u}} N_{\mathbf{u},j} = B\end{aligned}$$

is given in the following steps. We define

$$M_\mathbf{u}(\mu) = \prod_{j\in\mathbf{u}} \left(\frac{2s_{\mathbf{u},j} C_{\mathbf{u},j}}{\mu} \right)^{\frac{1}{2s_{\mathbf{u},j} + \sum_{k\in\mathbf{u}} s_{\mathbf{u},j}/s_{\mathbf{u},k}}}$$

and compute λ by $B = \sum_{\mathbf{u}\in U} M_\mathbf{u}(\lambda)$. Finally we get for $\mathbf{u} \in U$ and $j \in \mathbf{u}$

$$N_{\mathbf{u},j} = \sqrt{\frac{2s_{\mathbf{u},j} C_{\mathbf{u},j}}{\lambda M_\mathbf{u}(\lambda)}}^{\,1/s_{\mathbf{u},j}} \quad \text{and} \quad |\mathcal{I}_{\mathbf{N}_\mathbf{u}}| = M_\mathbf{u}(\lambda).$$

Algorithm

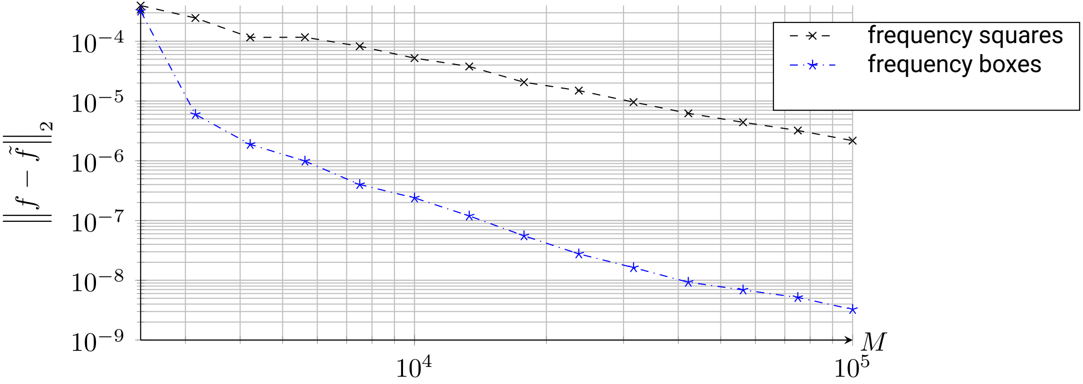
Input: • points $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_M\} \subset \mathbb{T}^d$, data $\mathbf{y} \in \mathbb{C}^M$
• initial index set $\mathcal{I}_0$, and frequency budget $B \in \mathbb{N}$

Output: approximation $\tilde{f} = \sum_{\mathbf{k}\in\mathcal{I}} \hat{f}_{\mathbf{k}} \exp(2\pi\mathrm{i}\,\langle \mathbf{k}, \cdot \rangle) \approx f$

compute approximated Fourier coefficients $\hat{f}_{\mathbf{k}},\ \mathbf{k} \in \mathcal{I}_0$ with $\mathcal{X}$ and $\mathbf{y} \in \mathbb{C}^M$ by least squares;
$\ell \leftarrow 0$;
repeat
    $\ell \leftarrow \ell + 1$;
    learn anisotropy $C_{\mathbf{u},j}$, and $s_{\mathbf{u},j}$ for all ANOVA terms based on $\hat{f}_{\mathbf{k}},\ \mathbf{k} \in \mathcal{I}_{\ell-1}$;
    update $\mathcal{I}_\ell$ based on $C_{\mathbf{u},j}$, and $s_{\mathbf{u},j}$ according to the theorem;
    compute updated approximated Fourier coefficients $\hat{f}_{\mathbf{k}},\ \mathbf{k} \in \mathcal{I}_\ell$ by least squares;
until *approximation good enough or step limit exceeded*;

Numerical Example

$$f(x_1, x_2, x_3) = b_6(x_1)b_2(x_3) + b_4(x_2)$$



Numerical Example

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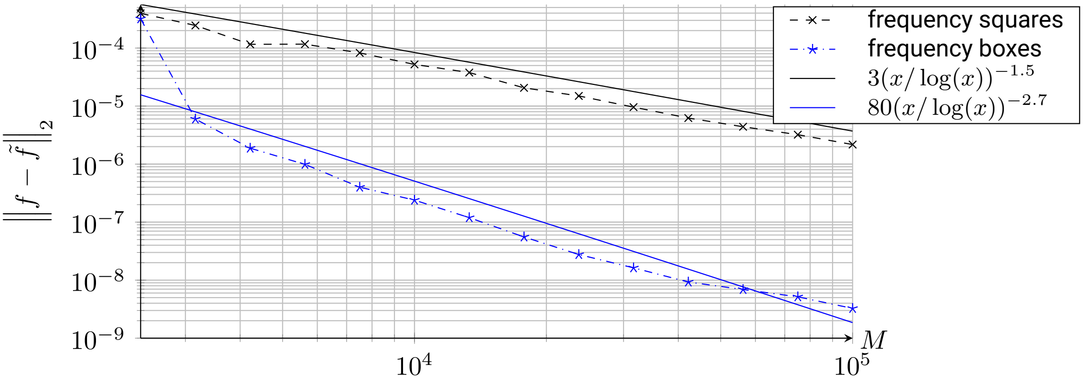

Conclusion

- We have an algorithm to learn anisotropy from computed Fourier coefficients
- We applied it for the ANOVA approximation to solve the parameter choice problem
- Preprint “Learning Anisotropy parameters in ANOVA approximation” is in preparation
- Outlook: Find optimal frequency budgets for noisy data using fast cross-validation[5]

[5] F. Bartel and R. Hielscher., **Concentration inequalities for cross-validation in scattered data approximation**, J. Approx. Theory, 227:Paper No. 105715, 17, (2022).

Conclusion

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Thank You

for Your attention

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Leave one out cross-validation

Let $\tilde{f}$ be an approximation based on data points and function values $\{(\mathbf{x}^1, y_1), \dots, (\mathbf{x}^M, y_M)\} \subset \mathbb{T}^d \times \mathbb{C}$ and $\tilde{f}_{-j}$ the same method on the samples with the j-th sample omitted. The cross-validation score is defined via

$$\text{CV}(\tilde{f}) = \frac{1}{n} \sum_{j=1}^{M} |\tilde{f}_{-j}(\mathbf{x}^j) - y_j|^2 .$$

Fast cross-validation

$$\text{FCV}(\tilde{f}) = \frac{1}{n} \sum_{j=1}^{M} \frac{|\tilde{f}(\mathbf{x}^j) - y_j|^2}{(1 - B/M)^2}$$