

Approximation with partially periodic basis functions in high dimensions

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UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Using d -dimensional function

$$f: \mathbb{T}^d \rightarrow \mathbb{C}, \mathbf{x} \mapsto f(\mathbf{x}).$$

Such functions can be written as a Fourier series

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} c_{\mathbf{k}}(f) \phi_{\mathbf{k}}(\mathbf{x}), \mathbf{x} \in \mathbb{T}^d$$

with Fourier basis functions $\phi_{\mathbf{k}}(\mathbf{x}) = \prod_{s=1}^d \exp(2\pi i k_s x_s)$ or alternatively with cosine basis functions.

Task

Given: $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_M\} \subset \mathbb{T}^d$ and $\mathbf{f} \in \mathbb{C}^M$ with $f(\mathbf{x}_j) = f_j, j = 1, \dots, M$

Goal: $\hat{f}_{\mathbf{k}} \approx c_{\mathbf{k}}(f) \in \mathbb{C}$, finite index set $\mathcal{I} \subset \mathbb{Z}^d$,

$$\text{such that } \tilde{f}(\mathbf{x}) := \sum_{\mathbf{k} \in \mathcal{I}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{x}) \approx f(\mathbf{x})$$

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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^①

$$\begin{aligned}
 f &= f_{\emptyset} && \dots 1 \times \text{constant function} \\
 &+ f_{\{1\}} + f_{\{2\}} + \dots + f_{\{d\}} && \dots d \times \text{univariate functions} \\
 &+ f_{\{1,2\}} + f_{\{1,3\}} + \dots + f_{\{d-1,d\}} && \dots \binom{d}{2} \times \text{bivariate functions} \\
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Outline

1. Motivation
2. Orthonormal basis
3. ANOVA decomposition
4. ANOVA approximation
5. Evaluation of Fourier cosine polynomials
6. Application
7. Conclusion

Fourier cosine basis functions

The functions

$$\phi_{\mathbf{k}}^{m,n} : \mathbb{T}^m \times [0, 1]^n \rightarrow \mathbb{C},$$

$$\phi_{\mathbf{k}}^{m,n}(\mathbf{x}) := \left(\prod_{s=1}^m \exp(2\pi i k_s x_s) \right) \cdot \left((\sqrt{2})^{|\text{supp}((k_j)_{j=m+1}^{m+n})|} \prod_{s=m+1}^{m+n} \cos(\pi k_s x_s) \right), \mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n$$

form an orthonormal basis of $L_2(\mathbb{T}^m \times [0, 1]^n)$.

Theorem

Every function $f \in L_2(\mathbb{T}^m \times [0, 1]^n)$ can be rewritten as

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n} c_{\mathbf{k}}(f) \phi_{\mathbf{k}}^{m,n}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{T}^m \times [0, 1]^n \text{ with the Fourier cosine coefficients}$$

$$c_{\mathbf{k}}(f) := \langle f, \phi_{\mathbf{k}}^{m,n} \rangle_{L_2(\mathbb{T}^m \times [0, 1]^n)}.$$

ANOVA terms

An ANOVA term is defined as

$$f_{\mathbf{u}}: \mathbb{T}^m \times [0, 1]^n \rightarrow \mathbb{C}, \quad f_{\mathbf{u}}(\mathbf{x}) := \sum_{\substack{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n \\ \text{supp } \mathbf{k} = \mathbf{u}}} c_{\mathbf{k}}(f) \phi_{\mathbf{k}}^{m,n}(\mathbf{x})$$

for a subset of indices $\mathbf{u} \subset \{1, \dots, m+n\}$.

$$f(\mathbf{x}) = \sum_{\mathbf{u} \in \mathcal{P}(\{1, \dots, m+n\})} f_{\mathbf{u}}(\mathbf{x})$$

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truncated ANOVA decomposition

We consider the truncated ANOVA decomposition

$$\mathbb{T}_U f = \sum_{\mathbf{u} \in U} f_{\mathbf{u}}$$

with $U \subseteq \mathcal{P}(\{1, \dots, m+n\})$, such that $\mathbb{T}_U f \approx f$ holds.

Example for $f: \mathbb{T}^m \times [0, 1]^n \rightarrow \mathbb{C}$ and $U = \{\mathbf{u} \in \mathcal{P}(\{1, \dots, d\}) \mid |\mathbf{u}| \leq 2\}$

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Variance

We define the variance of a function f as

$$\sigma^2(f) := \underbrace{\|f\|_{L_2(\mathbb{T}^m \times [0,1]^n)}^2}_{L_2 \text{ norm}} - \underbrace{|c_{\mathbf{0}}(f)|^2}_{\text{mean value}} = \sum_{\mathbf{k} \in (\mathbb{Z}^m \times \mathbb{N}_0^n) \setminus \{\mathbf{0}\}} |c_{\mathbf{k}}(f)|^2.$$

Global sensitivity indices^③

The global sensitivity index (GSI) of an ANOVA term $f_{\mathbf{u}}$ is defined as

$$\rho(\mathbf{u}, f) := \frac{\sigma^2(f_{\mathbf{u}})}{\sigma^2(f)}.$$

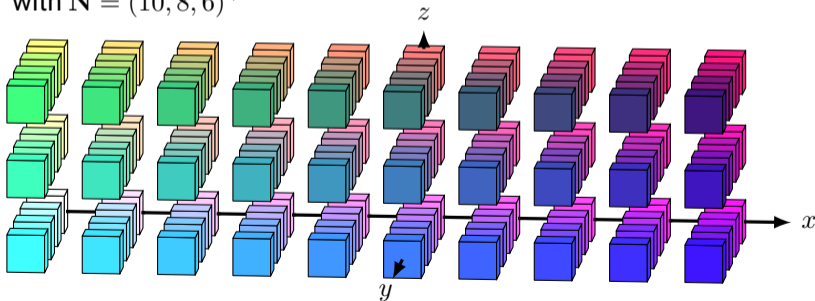
$$\sum_{\mathbf{u} \in \mathcal{P}(\{1, \dots, m+n\}) \setminus \{\emptyset\}} \rho(\mathbf{u}, f) = \frac{\sum_{\mathbf{u} \in \mathcal{P}(\{1, \dots, m+n\}) \setminus \{\emptyset\}} \sigma^2(f_{\mathbf{u}})}{\sigma^2(f)} = \frac{\sum_{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n \setminus \{\mathbf{0}\}} |c_{\mathbf{k}}(f)|^2}{\sum_{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n \setminus \{\mathbf{0}\}} |c_{\mathbf{k}}(f)|^2} = 1$$

^③Sobol, I. M., **Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates**, Math. Comput. Simulation, (2001).

Index set

$$\mathcal{I}_{\mathbf{N}}^{m,n} := \left\{ \mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n \mid k_j \geq -\frac{N_j}{2}, j = 1, \dots, m; \quad k_j < \frac{N_j}{2}, j = 1, \dots, m+n \right\}, \mathbf{N} \in (2\mathbb{N})^{m+n}$$

Example: $\mathcal{I}_{\mathbf{N}}^{1,2}$ with $\mathbf{N} = (10, 8, 6)^\top$



Fourier cosine polynomials

We define the set of Fourier cosine polynomials up to degree N as

$$\mathcal{T}_N := \left\{ \sum_{\mathbf{k} \in \mathcal{I}_N^{m,n}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n} \mid \hat{f}_{\mathbf{k}} \in \mathbb{C} \right\}.$$

Approximation

Given: $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_M\} \subseteq \mathbb{T}^m \times [0, 1]^n$ and $\mathbf{f} \in \mathbb{C}^M$ with $f(\mathbf{x}_j) = f_j, j = 1, \dots, M$

Goal: $\tilde{f} \in \mathcal{T}_N$ with $\tilde{f}(\mathbf{x}_j) \approx f_j, j = 1, \dots, M$

$$\Leftrightarrow \hat{\mathbf{f}} \in \mathbb{C}^{|\mathcal{I}_N^{m,n}|} \text{ with } \sum_{\mathbf{k} \in \mathcal{I}_N^{m,n}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j) \approx f_j, j = 1, \dots, M$$

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Approximation of the coefficients^②

$$\begin{aligned}
 \|f - \tilde{f}\|_{L_2(\mathbb{T}^m \times [0,1]^n)}^2 &= \int_{\mathbb{T}^m \times [0,1]^n} |f(\mathbf{x}) - \tilde{f}(\mathbf{x})|^2 d\mathbf{x} \\
 &\approx \frac{1}{|M|} \sum_{j=1}^M |f_j - \tilde{f}(\mathbf{x}_j)|^2 \\
 &= \frac{1}{|M|} \sum_{j=1}^M \left| f_j - \sum_{\mathbf{k} \in \mathcal{I}_{\mathbb{N}}^{m,n}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j) \right|^2 \\
 \hat{\mathbf{f}} &:= \arg \min_{\hat{\mathbf{h}} \in \mathbb{C}^{|\mathcal{I}_{\mathbb{N}}^{m,n}|}} \sum_{j=1}^M \left| f_j - \sum_{\mathbf{k} \in \mathcal{I}_{\mathbb{N}}^{m,n}} \hat{h}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j) \right|^2 \approx (c_{\mathbf{k}}(f))_{\mathbf{k} \in \mathcal{I}_{\mathbb{N}}^{m,n}}
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→ Least squares solver

^②Schmischke, M., **Interpretable Approximation of High-Dimensional Data based on the ANOVA Decomposition**, Thesis, Universitätsverlag Chemnitz, (2022).

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→ Least squares solver

^②Schmischke, M., **Interpretable Approximation of High-Dimensional Data based on the ANOVA Decomposition**, Thesis, Universitätsverlag Chemnitz, (2022).

Approximation of the coefficients^②

$$\begin{aligned}
 \|f - \tilde{f}\|_{L_2(\mathbb{T}^m \times [0,1]^n)}^2 &= \int_{\mathbb{T}^m \times [0,1]^n} |f(\mathbf{x}) - \tilde{f}(\mathbf{x})|^2 d\mathbf{x} \\
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Fourier cosine polynomials

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,n}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}), \hat{f} \in \mathbb{C}$$

Trigonometric polynomials

$$f^{\text{exp}}(\mathbf{x}) = \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,0}} \hat{f}_{\mathbf{k}}^{\text{exp}} \exp(2\pi i \langle \mathbf{k}, \mathbf{x} \rangle), \hat{f}^{\text{exp}} \in \mathbb{C}$$

The computation of the values $(f^{\text{exp}}(x_j))_{j=1}^M$ through a NFFT has the computational cost $O(|\mathcal{I}_{\mathbf{N}}^{m,0}| \log |\mathcal{I}_{\mathbf{N}}^{m,0}| + |\log \epsilon|^m M)$.

$$|\mathcal{I}_{\mathbf{N}}^{m,0}| = \prod_{j=1}^m N_j$$

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Theorem

Let $\hat{\mathbf{f}} = (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,n}} \in \mathbb{C}^{|\mathcal{I}_{\mathbf{N}}^{m,n}|}$ be a coefficient vector for a Fourier cosine polynomial f . We define a coefficient vector $\hat{\mathbf{f}}^{\text{exp}} = (\hat{f}_{\mathbf{k}}^{\text{exp}})_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m+n,0}} \in \mathbb{C}^{|\mathcal{I}_{\mathbf{N}}^{m+n,0}|}$ for a trigonometric polynomial f^{exp} through

$$\hat{f}_{\mathbf{k}}^{\text{exp}} := \begin{cases} 0 & , \exists j > m : k_j = -\frac{N_j}{2} \\ (\sqrt{2})^{-|\text{supp}(k_j)_{j=m+1}^{m+n}|} \hat{f}_{\left(\begin{smallmatrix} (k_j)_{j=1}^m \\ (|k_j|)_{j=m+1}^{m+n} \end{smallmatrix} \right)} & , \text{else} \end{cases} , \mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m+n,0}.$$

Then the following identity between the Fourier cosine polynomial f and the trigonometric polynomial f^{exp} holds

$$f(\mathbf{x}) = f^{\text{exp}} \left(\left(\begin{smallmatrix} (x_j)_{j=1}^m \\ (\frac{1}{2}x_j)_{j=m+1}^{m+n} \end{smallmatrix} \right) \right) \forall \mathbf{x} \in \mathbb{T}^m \times [0, 1]^n.$$

Remark

Fourier cosine polynomials can be evaluated thought a NFFT.

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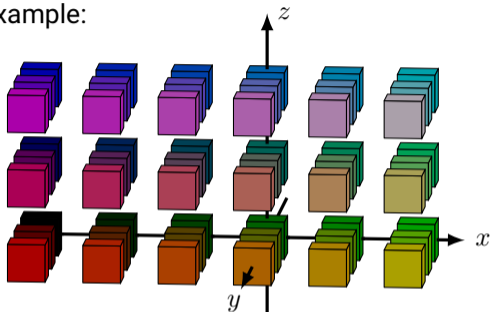
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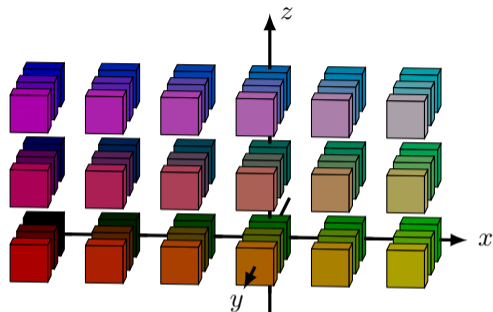
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Example:

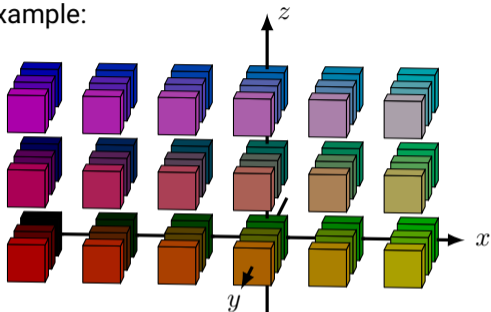


$$\mathcal{I}_{(6,6,6)}^{1,2}$$

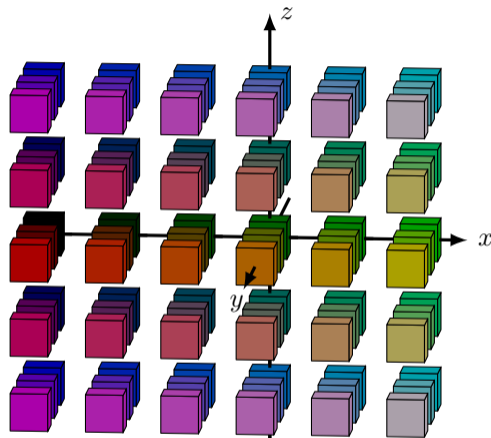


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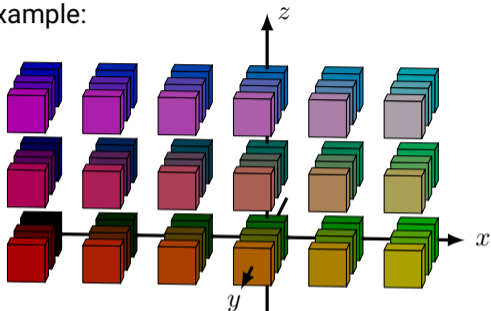


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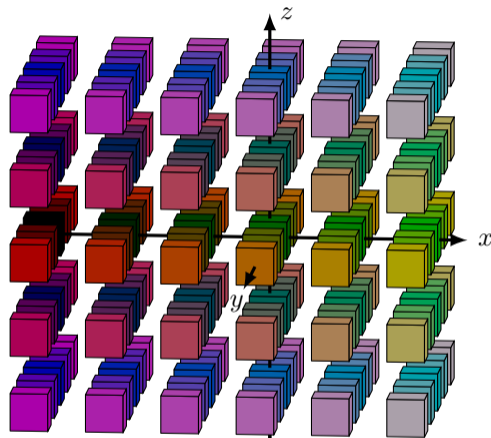


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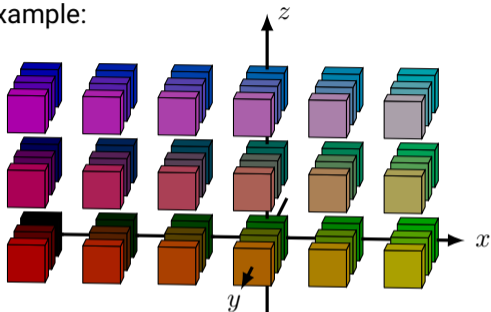


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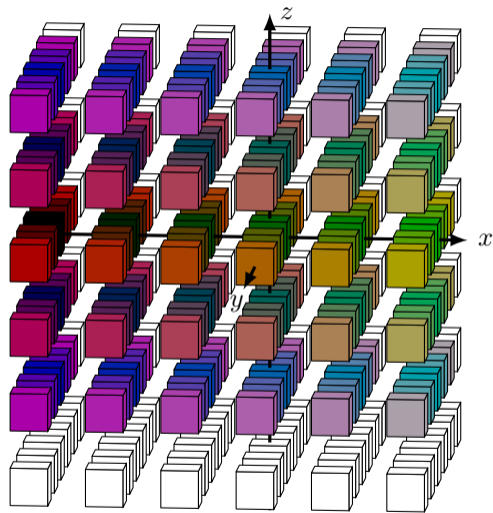


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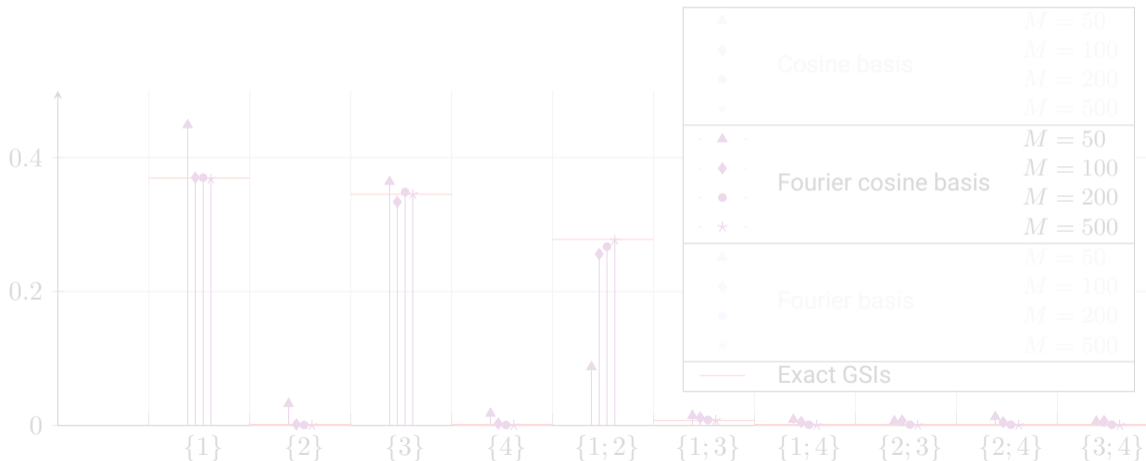


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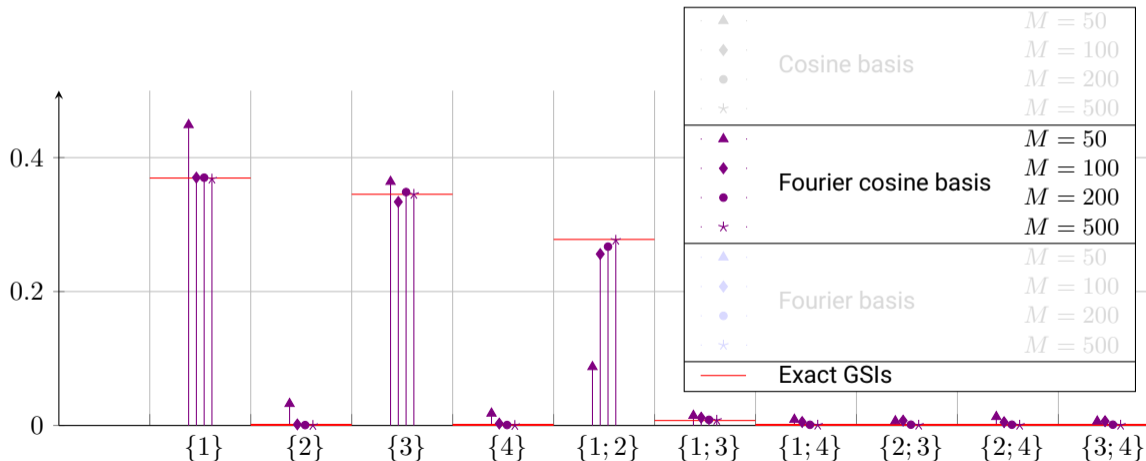


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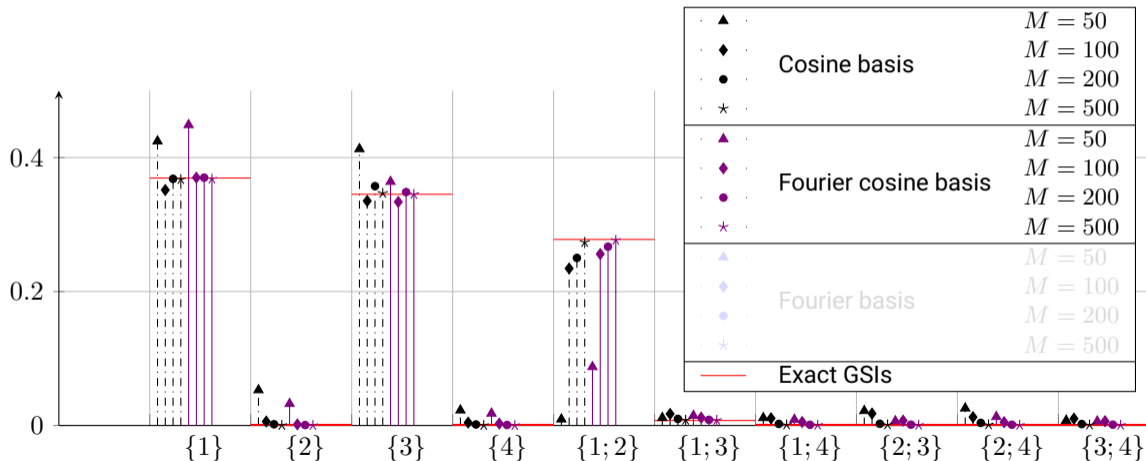
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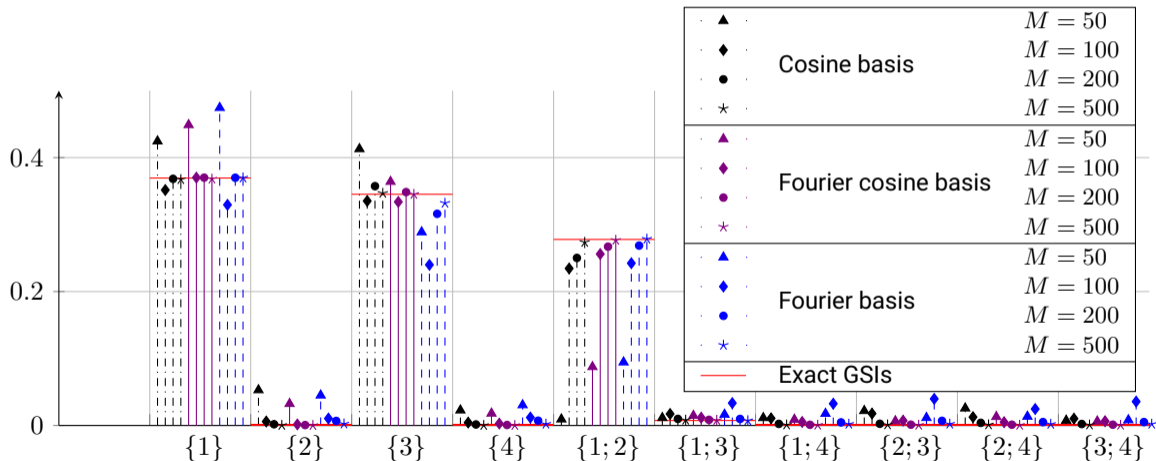
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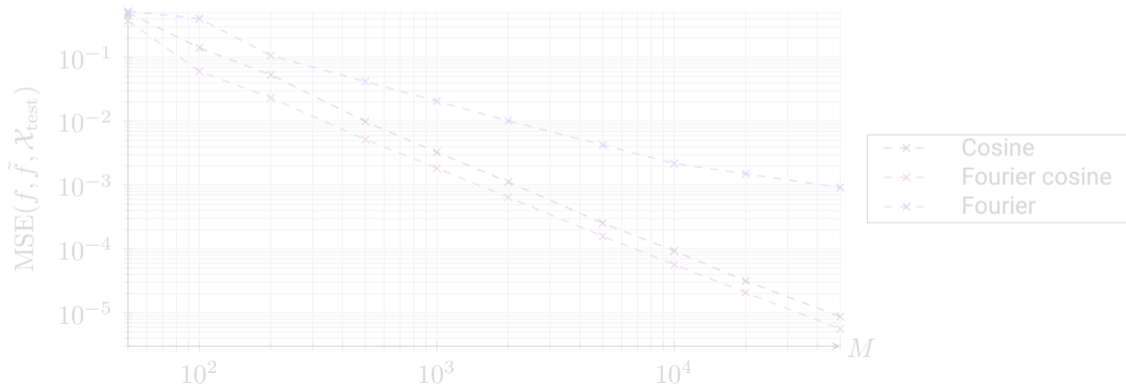


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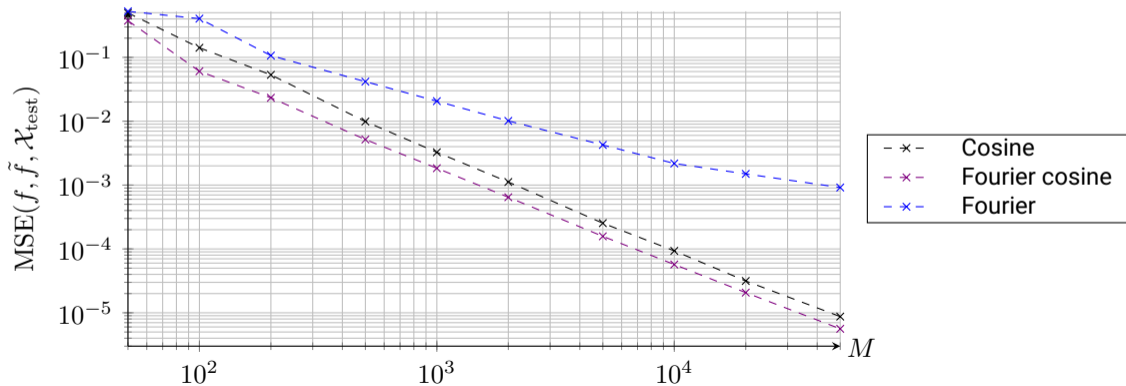
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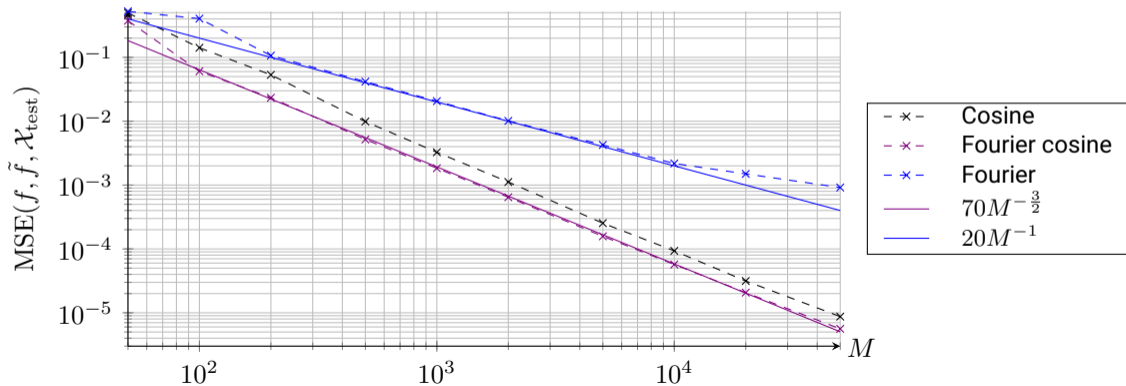
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Chebyshev basis functions

The functions

$$T_k: [0, 1] \rightarrow \mathbb{C},$$

$$T_k(x) := \cos(k \arccos(2x - 1)), \quad k \in \mathbb{N}_0$$

form an orthonormal basis of $L_2([0, 1], \omega)$ with the weight

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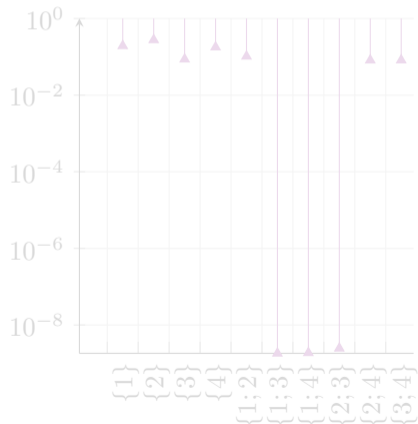
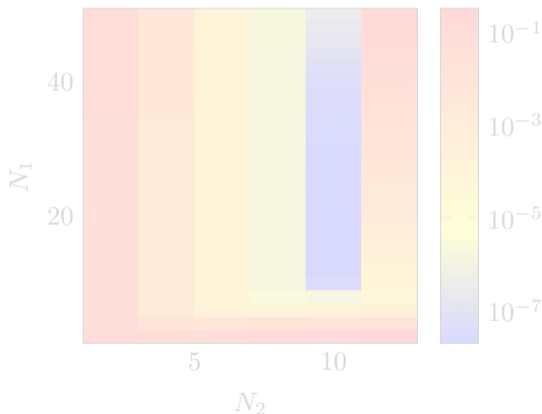
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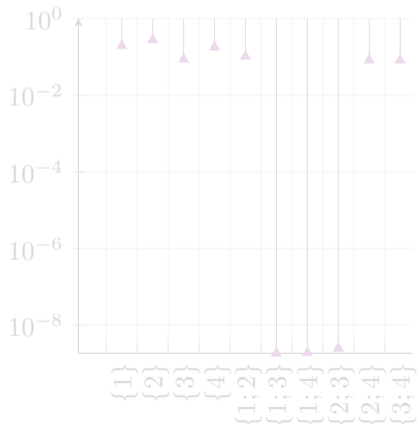
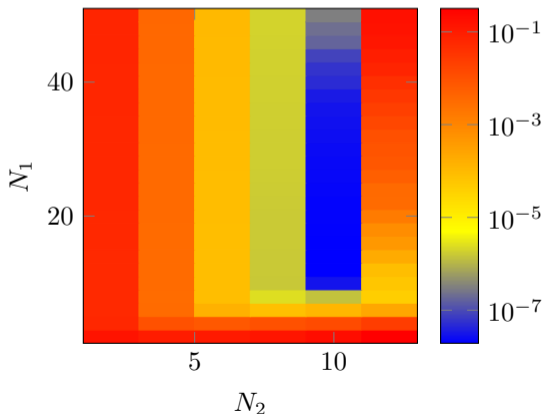
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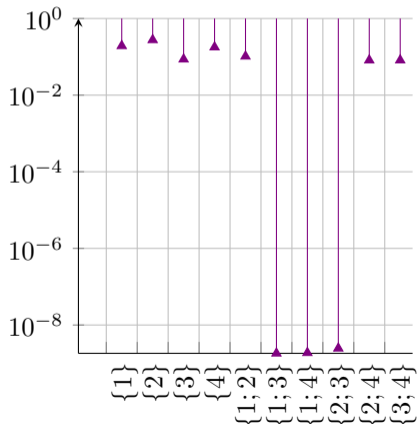
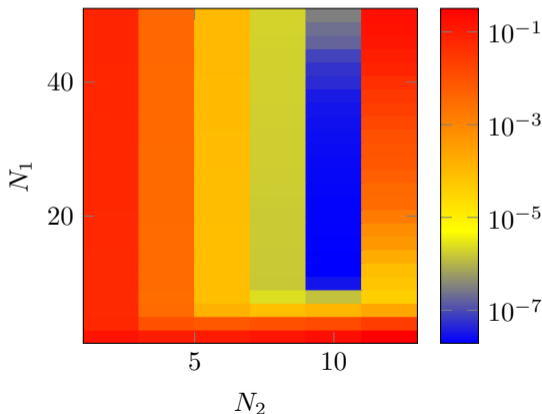
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Conclusion

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Thank You
for Your attention