High dimensional approximation with partially periodic boundary conditions

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Workshop on Mathematical Signal and Image Analysis

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UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Motivation

Using d-dimensional function

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

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

Task

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

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

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 terms①

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

$$\phi_{\mathbf{k}}^{m,n} \colon \mathbb{T}^m \times [0,1]^n \to \mathbb{C},$$
$$\phi_{\mathbf{k}}^{m,n}(\mathbf{x}) := \left(\prod_{s=1}^{m} \exp\left(2\pi \mathrm{i} k_s x_s\right)\right) \cdot \left(\left(\sqrt{2}\right)^{\left|\operatorname{supp}((k_j)_{j=m+1}^{m+n})\right|} \prod_{s=m+1}^{m+n} \cos\left(\pi k_s x_s\right)\right), \ \mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n$$

form an orthonormal basis of $\mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)$.

Theorem

Every function $f \in \mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)$ *can be rewritten as* $f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n} c_{\mathbf{k}}(f) \phi_{\mathbf{k}}^{m,n}(\mathbf{x}),\ \mathbf{x} \in \mathbb{T}^m \times [0,1]^n$ *with the Fourier cosine coefficients* $c_{\mathbf{k}}(f) := \langle f, \phi_{\mathbf{k}}^{m,n} \rangle_{\mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)}$.

ANOVA terms

An ANOVA term is defined as

$$f_{\mathbf{u}} \colon \mathrm{L}_2(\mathbb{T}^m \times [0,1]^n) \to \mathbb{C},\ f_{\mathbf{u}}(\mathbf{x}) := \sum_{\substack{\mathbf{k} \in \mathbb{Z}^m \times \mathbb{N}_0^n \\ \operatorname{supp} \mathbf{k} = \mathbf{u}}} c_{\mathbf{k}}(f) \phi_{\mathbf{k}}^{m,n}(\mathbf{x})$$

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

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

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

truncated ANOVA decomposition

We consider the truncated ANOVA decomposition

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

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

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

$$\begin{aligned} f = f_\emptyset &+ f_{\{1\}} + f_{\{2\}} + \dots + f_{\{d\}} \\ &+ f_{\{1,2\}} + f_{\{1,3\}} + \dots + f_{\{d-1,d\}} \\ &+ f_{\{1,2,3\}} + f_{\{1,2,4\}} + \dots + f_{\{d-2,d-1,d\}} \\ &\vdots \\ &+ f_{\{1,2,\dots,d\}} \end{aligned}$$

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Variance

We define the variance of a function f as

$$\sigma^2(f) := \underbrace{\|f\|^2_{\mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)}}_{\mathrm{L}_2 \text{ norm}} - \underbrace{|c_{\mathbf{0}}(f)|^2}_{\text{mean value}} = \sum_{\mathbf{k} \in (\mathbb{Z}^m \times \mathbb{N}_0^n) \setminus \{\mathbf{0}\}} |c_{\mathbf{k}}(f)|^2 .$$

Global sensitivity indices③

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

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

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

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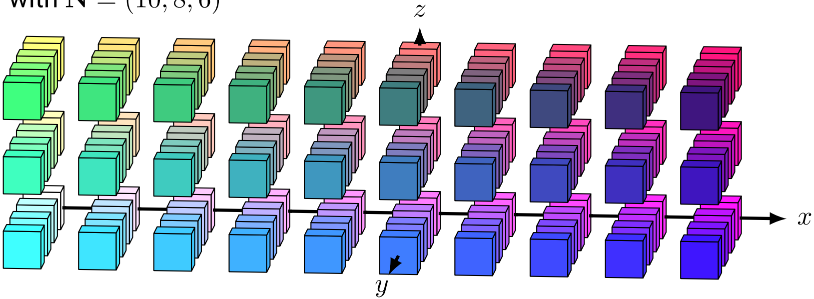
③ Sobol, I. M., **Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates**, Math. Comput. Simulation, (2001).

Index set

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

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 $\mathbf{N}$ as

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

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

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

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Approximation of the coefficients②

$$
\begin{aligned}
\left\| f - \tilde{f} \right\|^2_{\mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)} &= \int_{\mathbb{T}^m \times [0,1]^n} \left| f(\mathbf{x}) - \tilde{f}(\mathbf{x}) \right|^2 \mathrm{d}\mathbf{x} \\
&\approx \frac{1}{|M|} \sum_{j=1}^{M} \left| f_j - \tilde{f}(\mathbf{x}_j) \right|^2 \\
&= \frac{1}{|M|} \sum_{j=1}^{M} \left| f_j - \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,n}} \hat{f}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j) \right|^2
\end{aligned}
$$

$$
\hat{\mathbf{f}} := \operatorname*{arg\,min}_{\hat{\mathbf{h}} \in \mathbb{C}^{\left|\mathcal{I}_{\mathbf{N}}^{m,n}\right|}} \sum_{j=1}^{M} \left| f_j - \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,n}} \hat{h}_{\mathbf{k}} \phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j) \right|^2 \approx \left(c_{\mathbf{k}}(f)\right)_{\mathbf{k} \in \mathcal{I}_{\mathbf{N}}^{m,n}}
$$

→ Least squares solver

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

Approximation of the coefficients②

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$$\approx \frac{1}{|M|}\sum_{j=1}^{M}\left|f_j-\tilde{f}(\mathbf{x}_j)\right|^2$$

$$= \frac{1}{|M|}\sum_{j=1}^{M}\left|f_j-\sum_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}\hat{f}_{\mathbf{k}}\phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j)\right|^2$$

$$\hat{\mathbf{f}} := \underset{\hat{\mathbf{h}}\in\mathbb{C}^{\left|\mathcal{I}_{\mathbf{N}}^{m,n}\right|}}{\arg\min}\sum_{j=1}^{M}\left|f_j-\sum_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}\hat{h}_{\mathbf{k}}\phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j)\right|^2 \approx \left(c_{\mathbf{k}}(f)\right)_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}$$

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Approximation of the coefficients②

$$\begin{aligned}\left\|f-\tilde{f}\right\|^2_{\mathrm{L}_2(\mathbb{T}^m\times[0,1]^n)} &= \int_{\mathbb{T}^m\times[0,1]^n} \left|f(\mathbf{x})-\tilde{f}(\mathbf{x})\right|^2 \,\mathrm{d}\mathbf{x} \\ &\approx \frac{1}{|M|}\sum_{j=1}^{M}\left|f_j-\tilde{f}(\mathbf{x}_j)\right|^2 \\ &= \frac{1}{|M|}\sum_{j=1}^{M}\left|f_j-\sum_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}\hat{f}_{\mathbf{k}}\phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j)\right|^2\end{aligned}$$

$$\hat{\mathbf{f}} := \operatorname*{arg\,min}_{\hat{\mathbf{h}}\in\mathbb{C}^{\left|\mathcal{I}_{\mathbf{N}}^{m,n}\right|}} \sum_{j=1}^{M}\left|f_j-\sum_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}\hat{h}_{\mathbf{k}}\phi_{\mathbf{k}}^{m,n}(\mathbf{x}_j)\right|^2 \approx \left(c_{\mathbf{k}}(f)\right)_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m,n}}$$

→ Least squares solver

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

Approximation of the coefficients②

$$
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\left\| f - \tilde{f} \right\|^2_{\mathrm{L}_2(\mathbb{T}^m \times [0,1]^n)} &= \int_{\mathbb{T}^m \times [0,1]^n} \left| f(\mathbf{x}) - \tilde{f}(\mathbf{x}) \right|^2 \, \mathrm{d}\mathbf{x} \\
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\end{aligned}
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② Schmischke, M., **Interpretable Approximation of High-Dimensional Data based on the ANOVA Decomposition**, Thesis, Universitätsverlag Chemnitz, (2022).

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

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

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

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

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Evaluation of Fourier cosine polynomials

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* $\hat{\mathbf{f}}^{\exp} = (\hat{f}_{\mathbf{k}}^{\exp})_{\mathbf{k}\in\mathcal{I}_{\mathbf{N}}^{m+n,0}} \in \mathbb{C}^{|\mathcal{I}_{\mathbf{N}}^{m+n,0}|}$ *for a trigonometric polynomial* $f^{\exp}$ *through*

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

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

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

Remark

Fourier cosine polynomials can be evaluated thought a NFFT.

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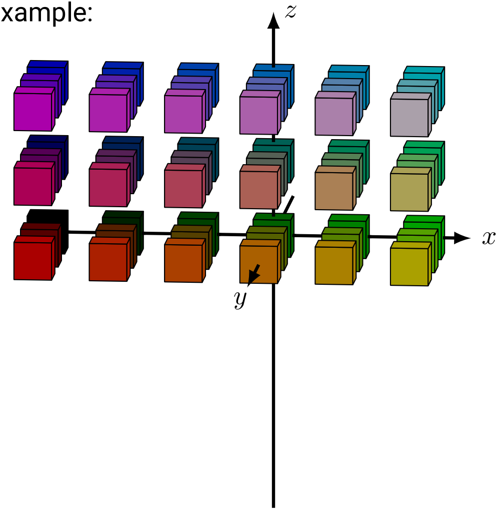
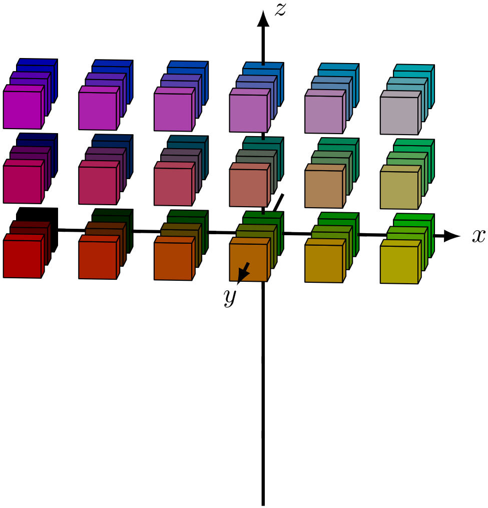
Fourier cosine polynomials can be evaluated thought a NFFT.

Example:



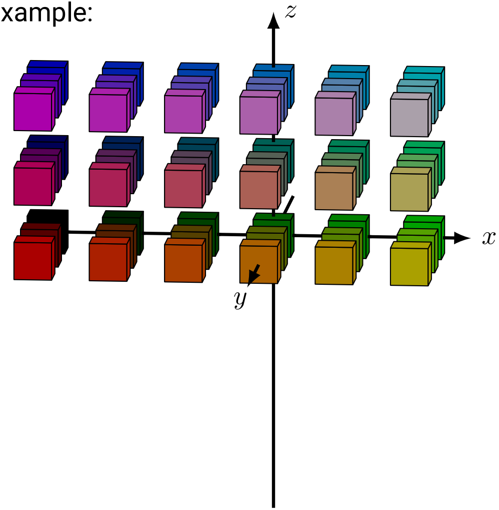
$\mathcal{I}^{1,2}_{(6,6,6)^\top}$



$\mathcal{I}^{3,0}_{(6,6,6)^\top}$

Evaluation of Fourier cosine polynomials

Example:



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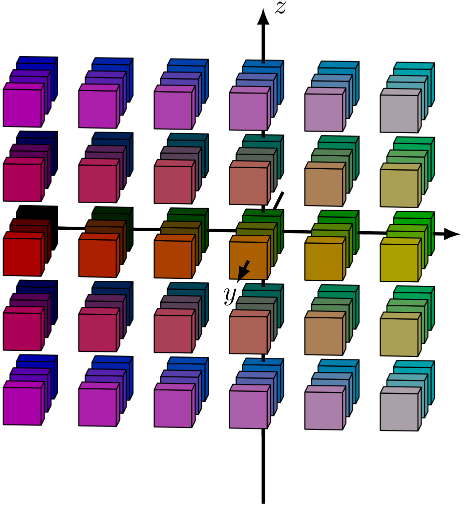

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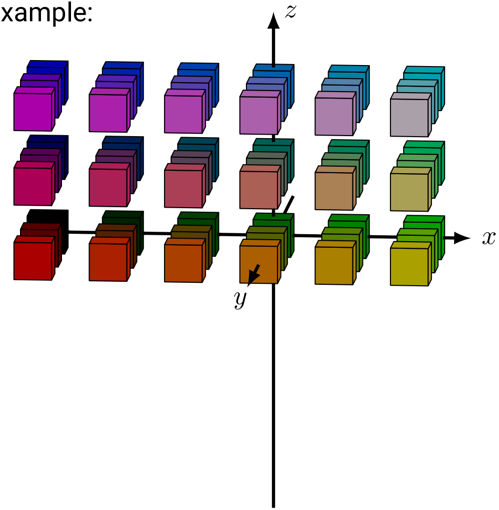
Example:



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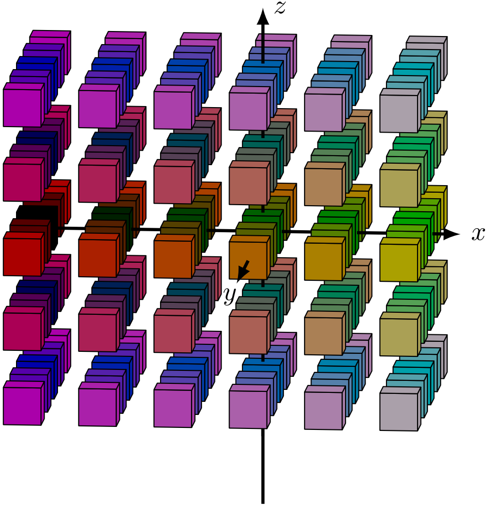

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Evaluation of Fourier cosine polynomials

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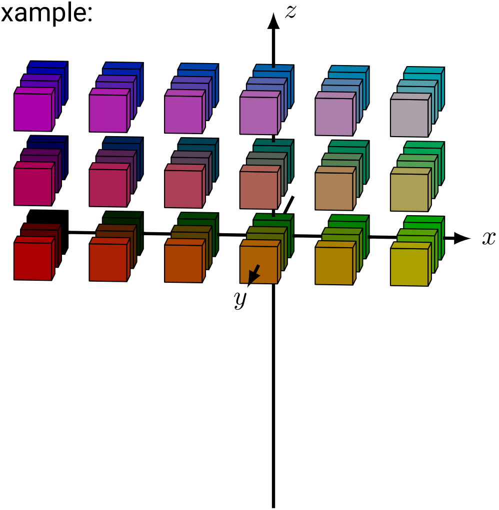

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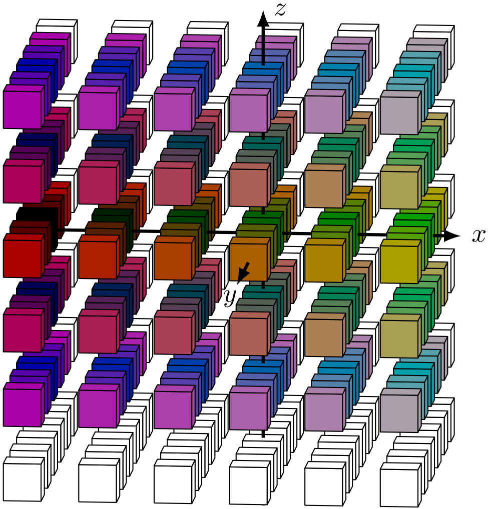

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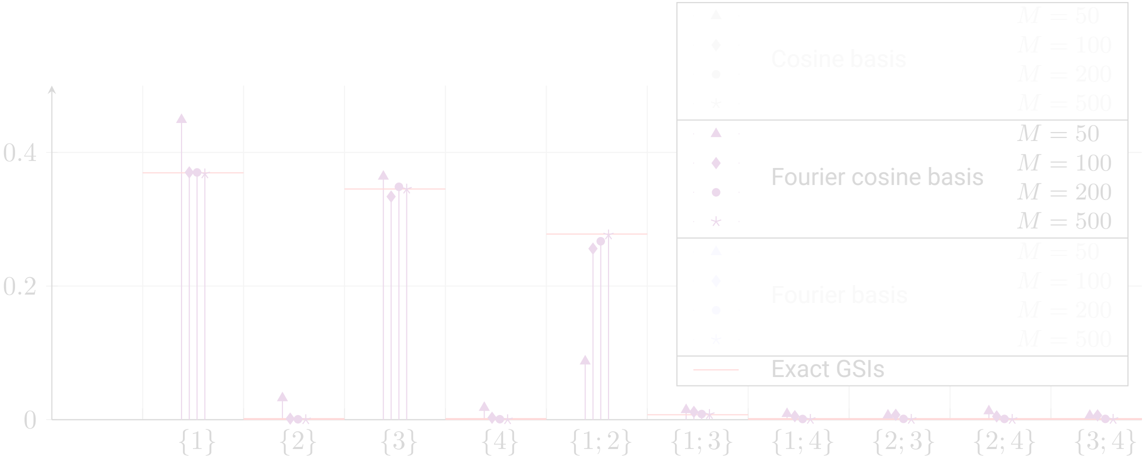
Application

$$f\colon [0,1]^4 \to \mathbb{C},\ f(x_1,x_2,x_3,x_4) \coloneqq (2x_1-1)^2 x_3 + 10\sin(2\pi x_1)\left(x_2-\frac{1}{2}\right)^2 + \exp(x_3)$$



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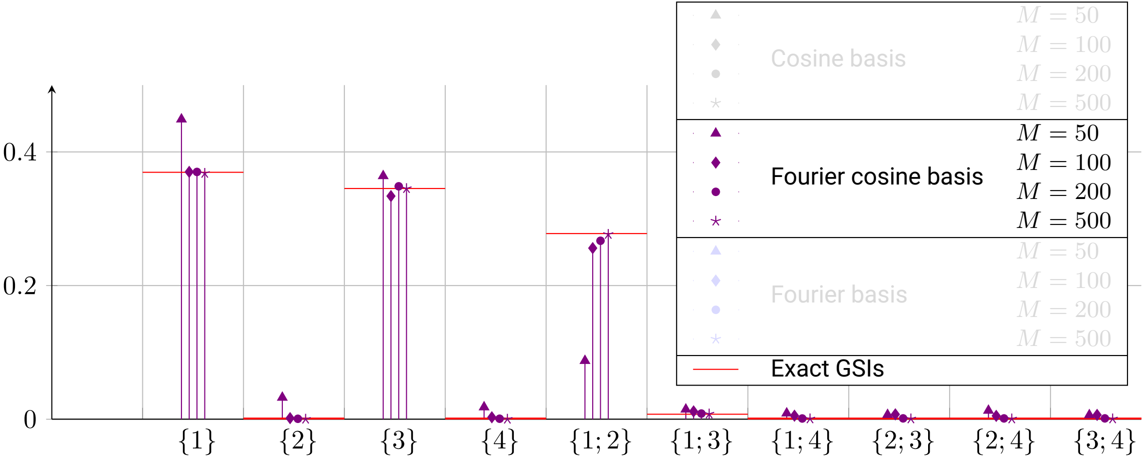

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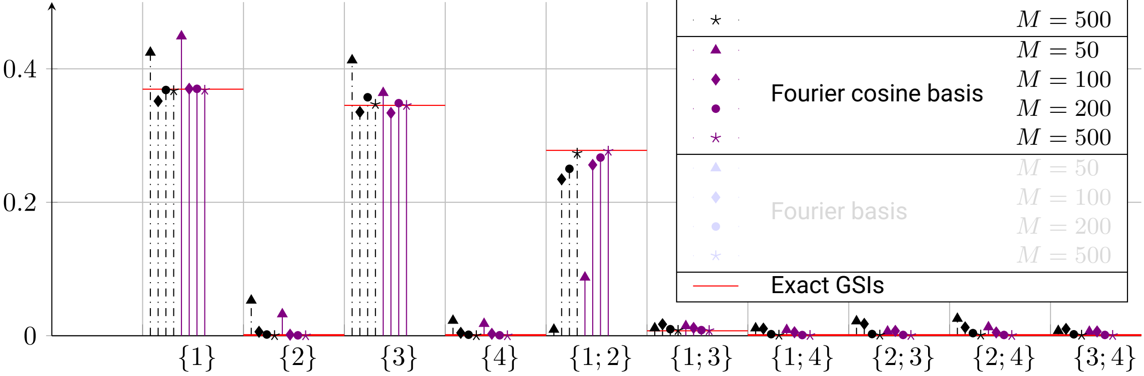

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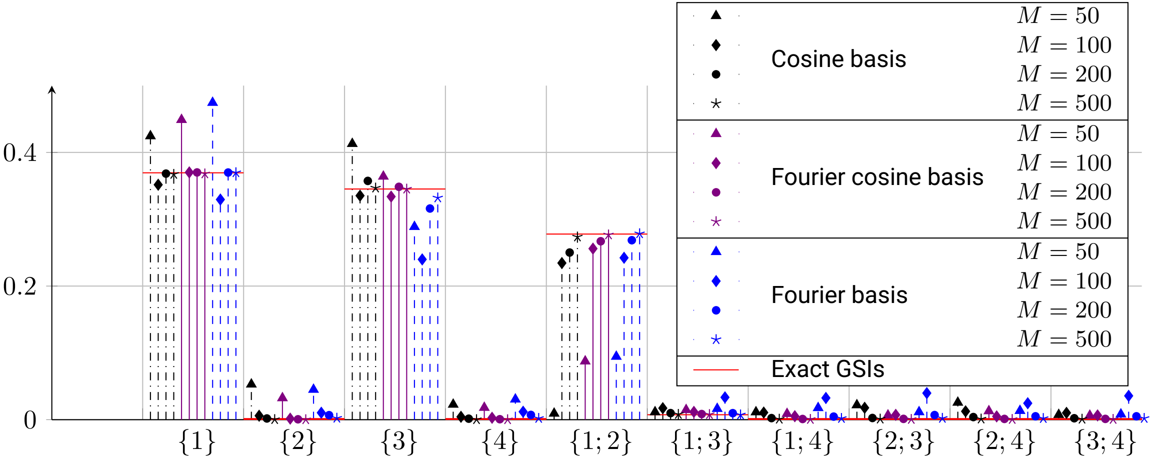

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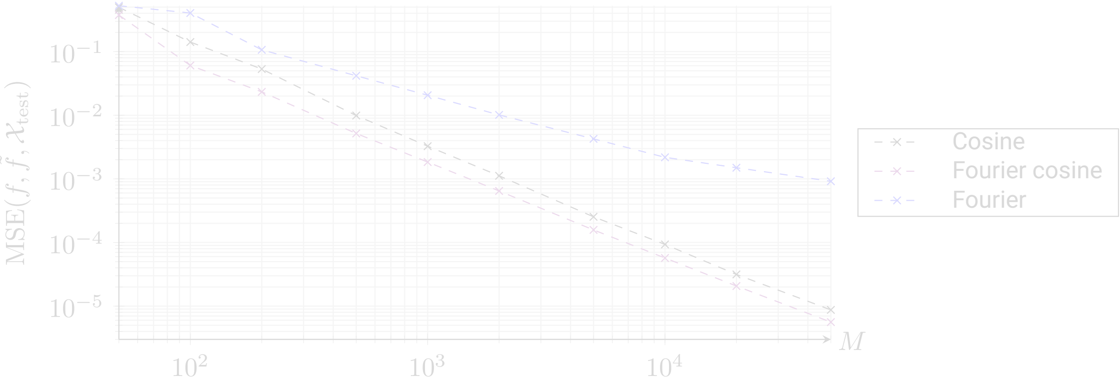

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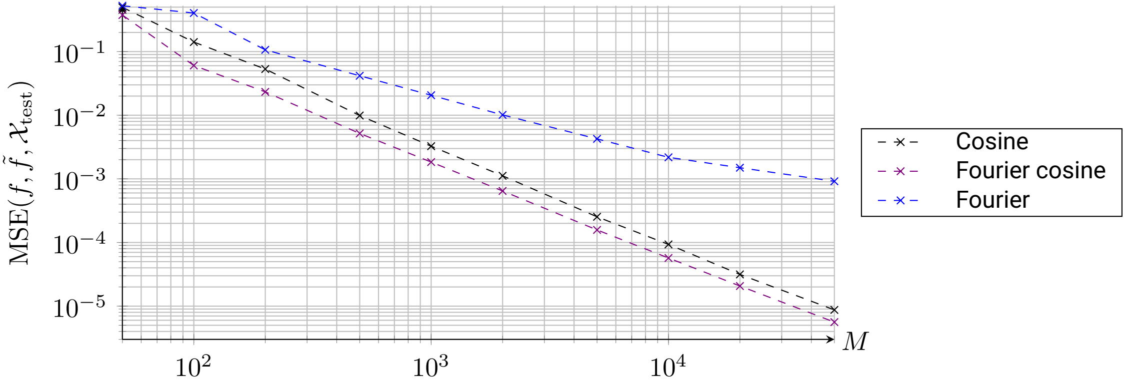

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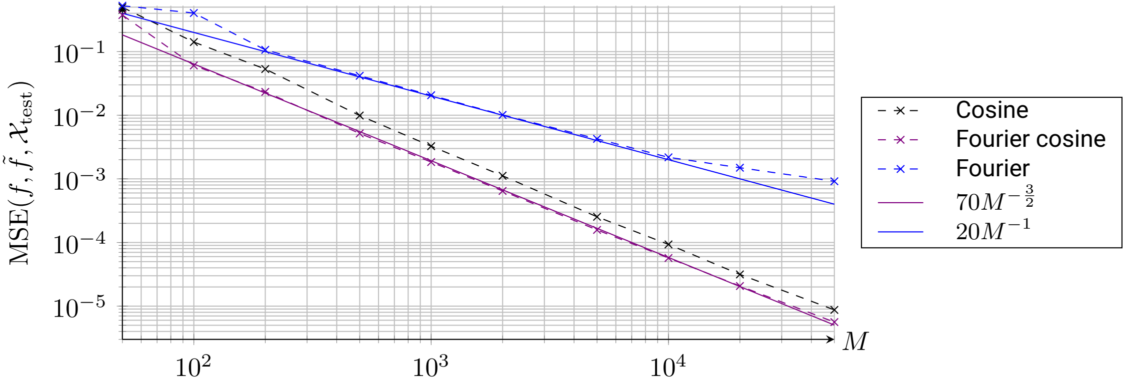

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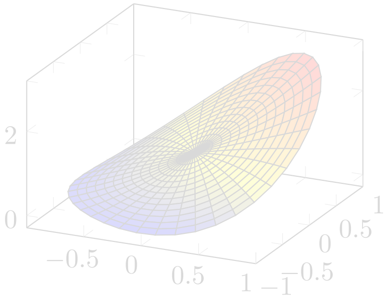

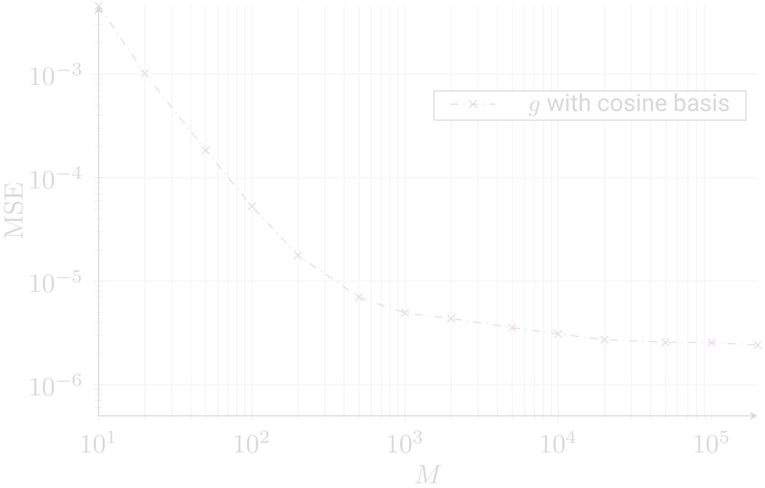

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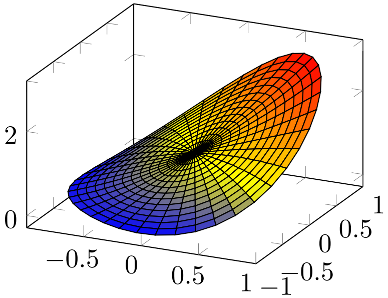

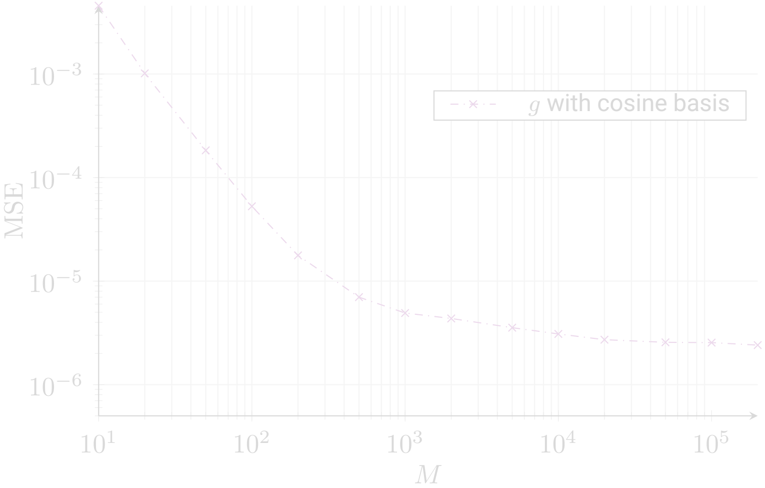

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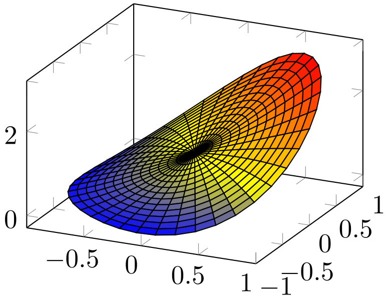

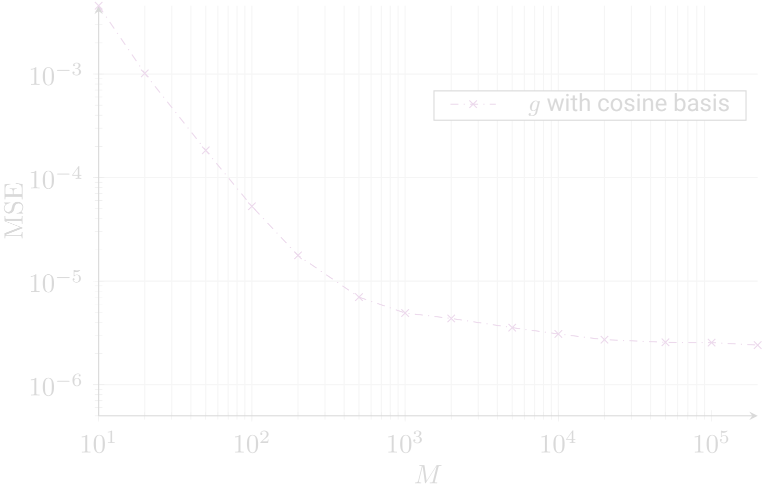

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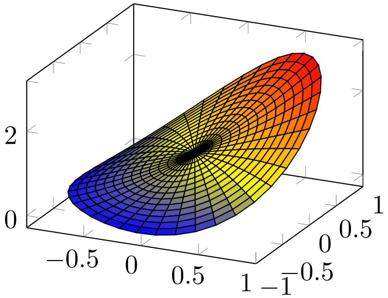

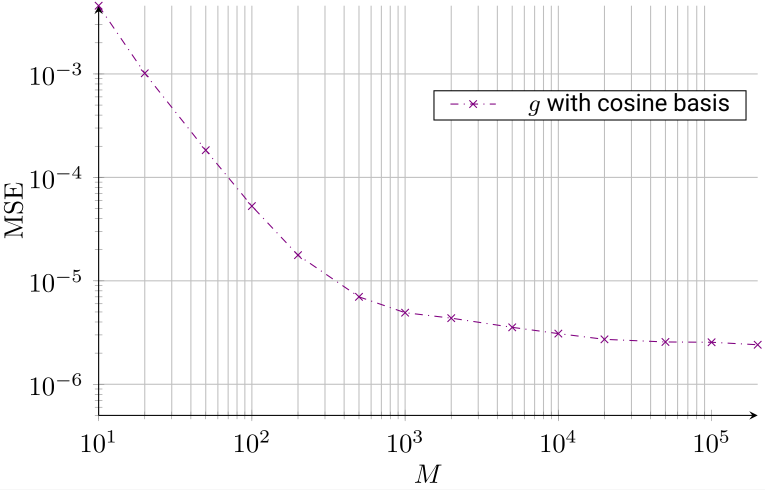

Polar coordinates

$$t\colon \mathbb{T}\times[0,1]\to\mathbb{B}^2,$$
$$t(\mathbf{x}) := (x_2\cos(2\pi x_1), x_2\sin(2\pi x_1))$$

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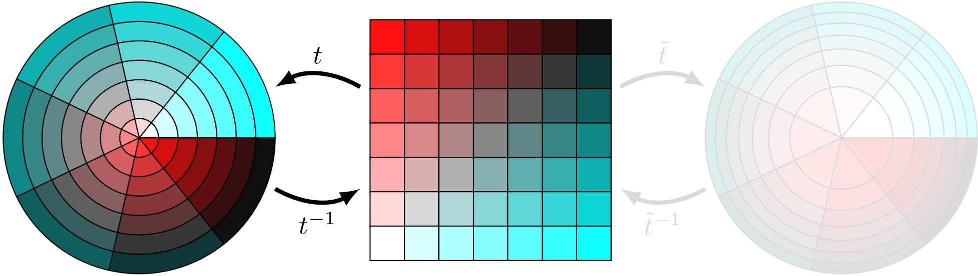

Basis on the disc

The functions $\phi_{\mathbf{k}}^{\mathbb{B}^2} := \sqrt{2}\phi_{\mathbf{k}}^{1,1}\circ\tilde{t}^{-1}\colon \mathbb{B}^2\to\mathbb{C}$, $\mathbf{k}\in\mathbb{Z}\times\mathbb{N}_0$ are an orthonormal basis of $\mathrm{L}_2(\mathbb{B}^2)$.

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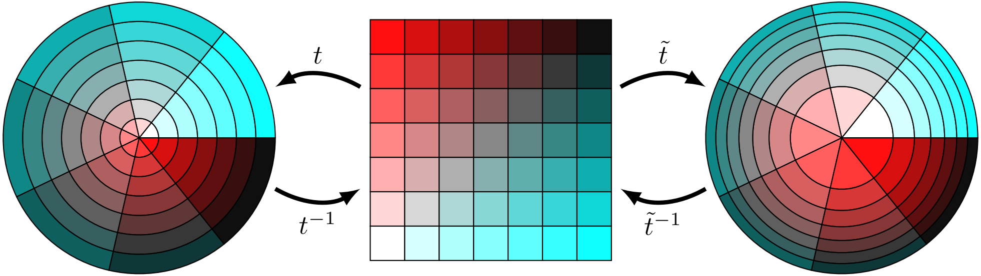

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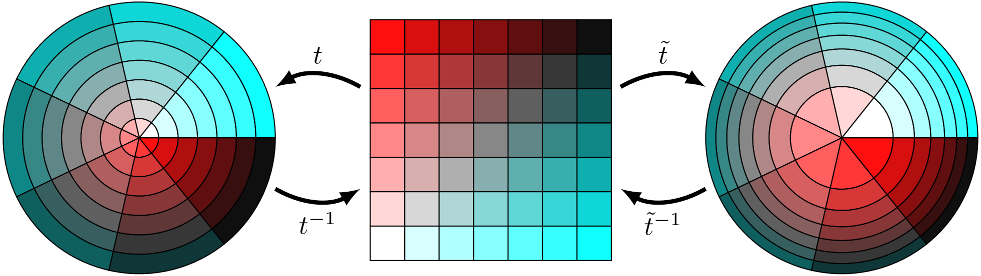

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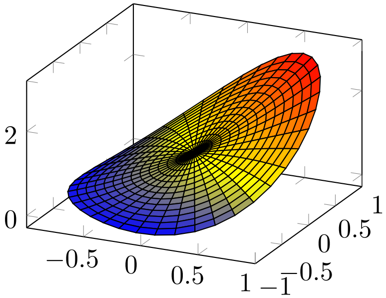

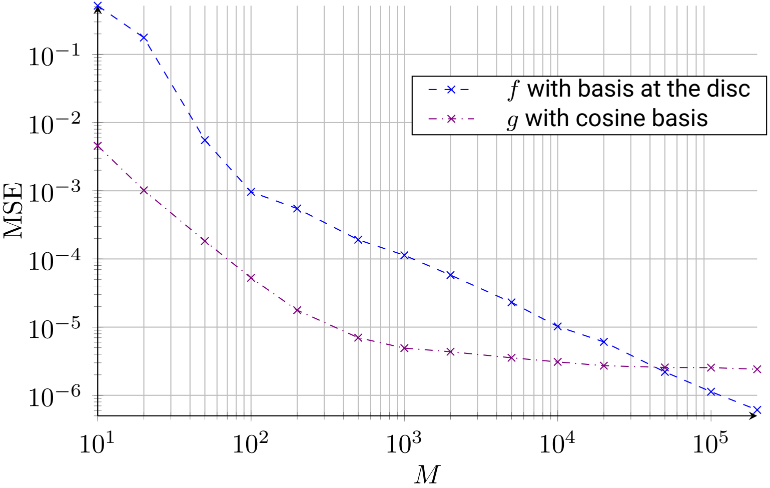

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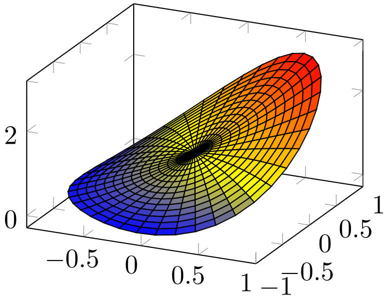

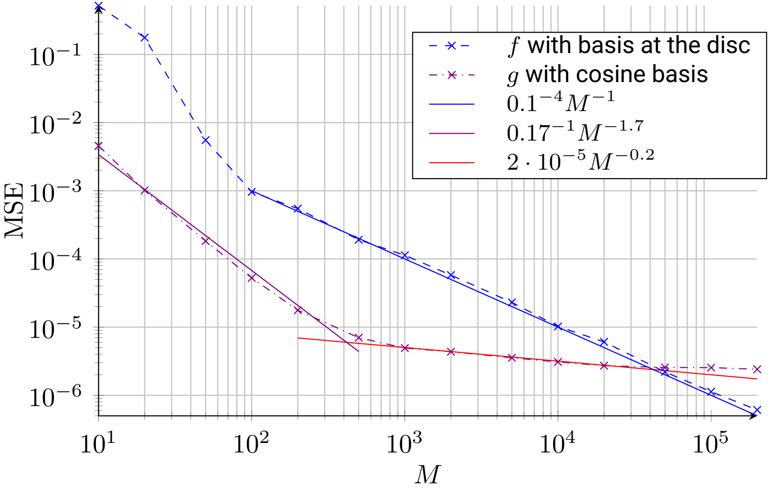

Conclusion

- We can approximate partial periodic functions $f\colon \mathbb{T}^m \times [0,1]^n \to \mathbb{C}$
- This is fast for functions with mainly low dimensional interactions
- It is implemented in the ANOVA framework as Branch named NFFCT
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- Outlook: approximate functions on $\mathbb{B}^d$ and $\mathbb{S}^d$

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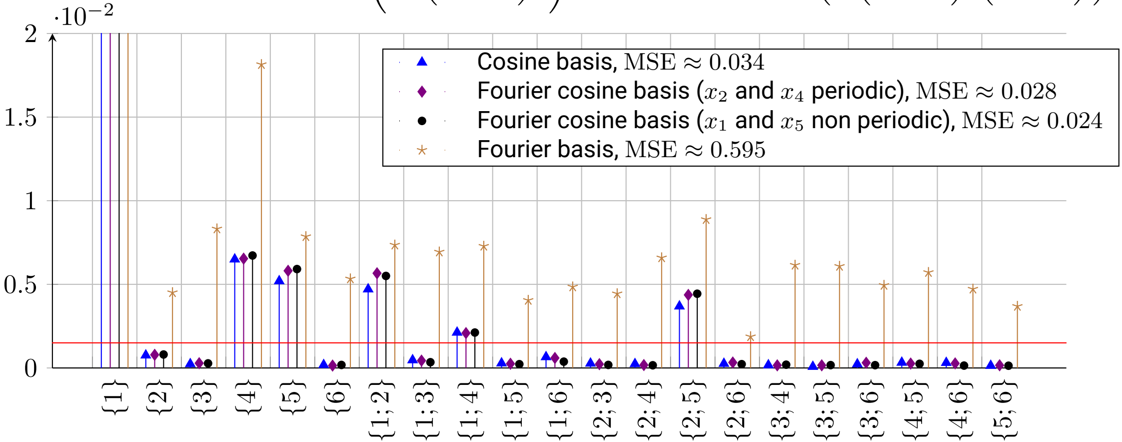
Thank You

for Your attention

Application

$$f\colon [0,1]^6 \to \mathbb{C},\ f(\mathbf{x}) := 5x_1^2 + 3\left(x_1^2\left(x_2-\frac{1}{2}\right)^2\right)^3 + \sin(x_1x_4) + 4\cos\left(\pi\left(x_2-\frac{1}{2}\right)\left(x_5-\frac{1}{2}\right)\right)$$



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$\mathrm{MSE}(f_1, \tilde{f}_1, \mathcal{X}_{\text{test}})$				x_1			
				cos		exp	
				x_2		x_2	
				cos	exp	exp	cos
x_4	cos	x_5	cos	0.01995	0.01496	0.33073	0.33592
			exp	0.01971	**0.01457**	0.33329	0.33557
	exp	x_5	exp	0.02385	0.01873	0.32361	0.33935
			cos	0.02409	0.01927	0.33555	0.33948