Learning the solution of differential equations by sparse high-dimensional approximation

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joint work with Lutz Kämmerer and Daniel Potts

Special Session: Function recovery and discretization problems

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UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Differential problem

$$Lu = f \qquad \boldsymbol{x} \in \Omega \subset \mathbb{R}^d$$

- differential operator L, domain Ω
- source term $f(\boldsymbol{x})$, solution $u(\boldsymbol{x})$
- **solution mapping $G(f) = u$**

Parametrization of f

$$f(\boldsymbol{x}) \approx \sum_{j=1}^{n} a_j A_j(\boldsymbol{x}) \qquad \boldsymbol{x} \in \Omega$$

- fixed functions $A_j, j = 1, \ldots, n$ (B-splines, trig. polynomials, ...)
- identify f by coefficients $\boldsymbol{a} \in \mathbb{C}^n$

Basis expansion of u in a bounded orthonormal product basis

$$u(\boldsymbol{x}, \boldsymbol{a}) := \sum_{\boldsymbol{k} \in \mathbb{N}^{d+n}} c_{\boldsymbol{k}} \Phi_{\boldsymbol{k}}(\boldsymbol{x}, \boldsymbol{a})$$

- coefficients $c_{\boldsymbol{k}} \in \mathbb{C}$ and functions $\Phi_{\boldsymbol{k}}(\cdot)$ bounded, orthonormal and of tensor-product structure

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High-dimensional approximation problem

$$S_I u(\boldsymbol{x},\boldsymbol{a}) := \sum_{\boldsymbol{k}\in I} \hat{u}_{\boldsymbol{k}} \Phi_{\boldsymbol{k}}(\boldsymbol{x},\boldsymbol{a})$$

- **index set:** $I \subset \mathbb{N}^{d+n}$ unknown but s-sparse ($|I| = s$)
- **coefficients:** $\hat{u}_{\boldsymbol{k}} \in \mathbb{C}$ approximations of true coefficients $c_{\boldsymbol{k}}$

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Benefits: The structure of the detected index set I contains various information about the solution and its dependence on $\boldsymbol{x}$ and f!
Problem: How to find a good, s-sparse index set I?

- first idea:
  - choose a large search space $\Gamma \supset \mathrm{I}, |\Gamma| \gg |\mathrm{I}|$
  - compute all coefficients $\hat{u}_{\boldsymbol{k}}$
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- but: unfeasible in practice for large Γ ($\rightarrow$ "curse of dimensionality")
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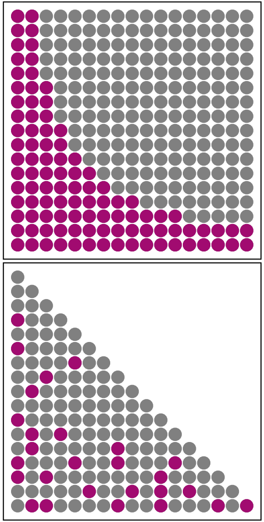

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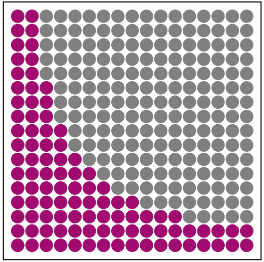

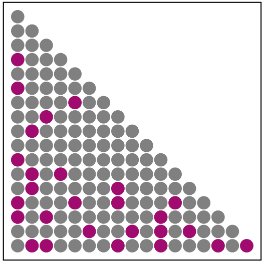

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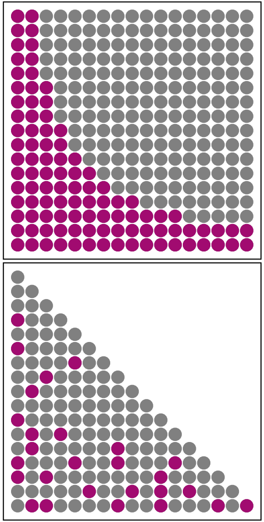

Differential equation setting

- approximate $u(\boldsymbol{x}, \boldsymbol{a})$ with $(\boldsymbol{x}, \boldsymbol{a}) \in \mathbb{R}^{d+n}$
- compute $I \subset \mathbb{N}^{d+n}$ and $\hat{u}_{\boldsymbol{k}}$ for $\boldsymbol{k} \in I$

$\longleftrightarrow$

Function approximation setting

- approximate $g(\boldsymbol{y})$ with $\boldsymbol{y} \in \mathbb{R}^d$
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Input

- target function g (black box)
- search space $\Gamma \subset \mathbb{N}^d$
- sparsity $s \in \mathbb{N}$
- detection threshold $\delta_+ > 0$
- number of detection iterations $r \in \mathbb{N}$

$\longrightarrow$

Output

- detected index set $I \subset \mathbb{N}^d$ with $|I| = s$
- approximated coefficients $\hat{g}_{\boldsymbol{k}}$ for $\boldsymbol{k} \in I$

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Projected coefficients

$$c_{\{1,\dots,t\},\boldsymbol{k}}(\tilde{\boldsymbol{y}}) \coloneqq \int_{\mathcal{D}_{\{1,\dots,t\}}} g(\boldsymbol{\xi}, \tilde{\boldsymbol{y}}) \, \overline{\Phi_{\{1,\dots,t\},\boldsymbol{k}}(\boldsymbol{\xi})} \, \mathrm{d}\mu_{\{1,\dots,t\}}(\boldsymbol{\xi}) \qquad \forall \boldsymbol{k} \in \mathbb{N}^t, \ \forall \tilde{\boldsymbol{y}} \in \mathcal{D}_{\{t+1,\dots,d\}}$$

Projected coefficients are similar to basis coefficients $c_{\boldsymbol{k}}$, but:

- fix some dimensions via a random anchor $\tilde{\boldsymbol{y}}$
- integrate only over the remaining dimensions

Projected coefficients indicate the "importance" of the indices $(\boldsymbol{k}, *, *, *, \dots)$, since

$$c_{\{1,\dots,t\},\boldsymbol{k}}(\tilde{\boldsymbol{y}}) = \dots = \sum_{\boldsymbol{h} \in \mathbb{N}^{d-t}} c_{(\boldsymbol{k},\boldsymbol{h})} \Phi_{\{t+1,\dots,d\},(\boldsymbol{k},\boldsymbol{h})}(\tilde{\boldsymbol{y}}).$$

Example: Fourier setting with $d = 3$ and $t = 2$

$$c_{\{1,2\},\boldsymbol{k}}(\tilde{y}) \coloneqq \int_{\mathbb{T}^2} g(\boldsymbol{\xi}, \tilde{y}) \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{\xi}} \, \mathrm{d}\boldsymbol{\xi} = \sum_{h \in \mathbb{Z}} c_{(\boldsymbol{k},h)} \mathrm{e}^{2\pi \mathrm{i} h \tilde{y}} \qquad \forall \boldsymbol{k} \in \mathbb{Z}^2, \ \forall \tilde{y} \in \mathbb{T}$$

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Approximation of projected coefficients

use any method for numerical integration, e.g., MC or QMC methods

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Properties of the approximation $\Longleftrightarrow$ Properties of the algorithm

fast approximation of proj. coef.	$\Longleftrightarrow$	fast algorithm
sample efficient approximation of proj. coef.	$\Longleftrightarrow$	sample efficient algorithm
accurate approximation of proj. coef.	$\Longleftrightarrow$	accurate algorithm

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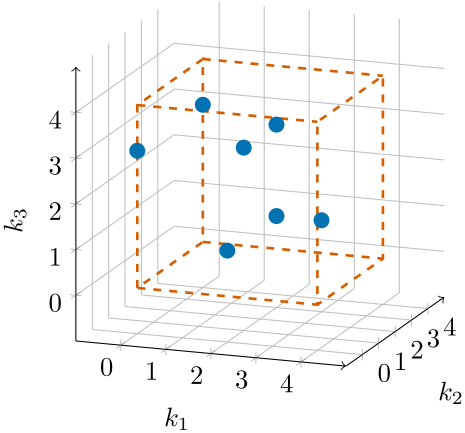
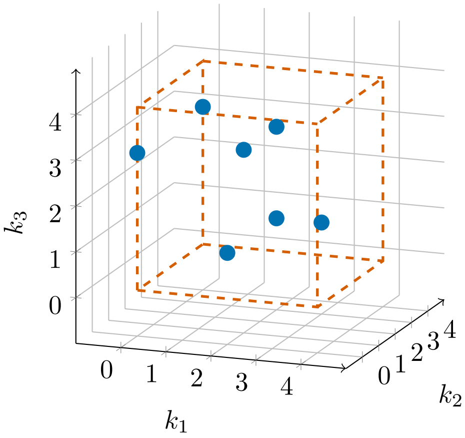


Figure: The desired but unknown index set I and the search space $\Gamma = \{0, 1, 2, 3, 4\}^3$.



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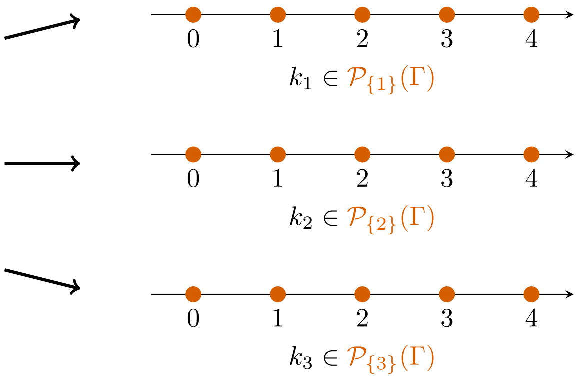


Figure: The one-dimensional candidate sets $\mathcal{P}_{\{j\}}(\Gamma)$.

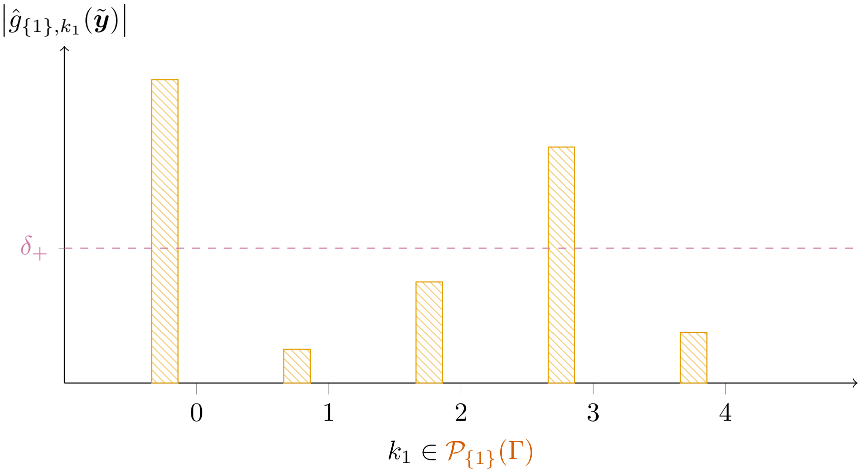
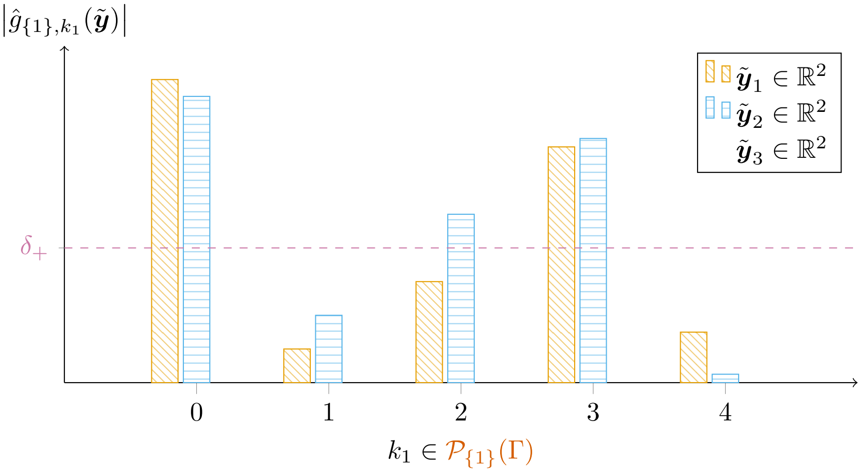


Figure: The one-dimensional detection step in the first dimension with $r = 3$ detection iterations.



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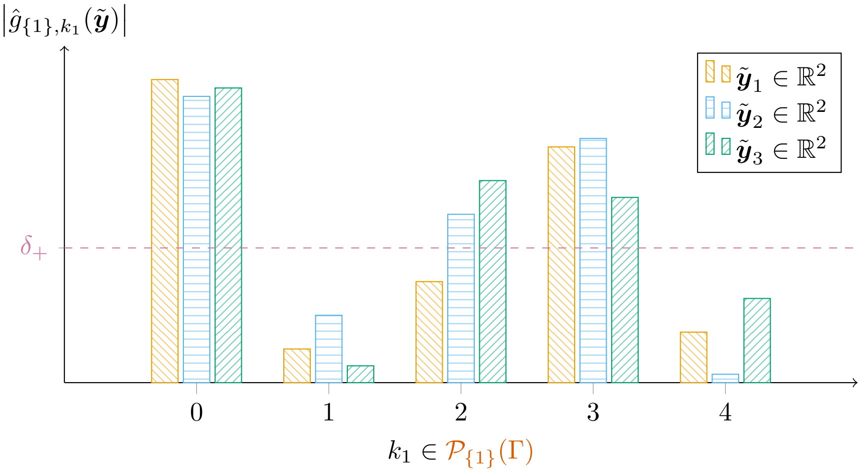

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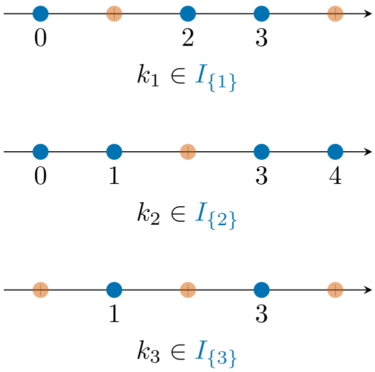
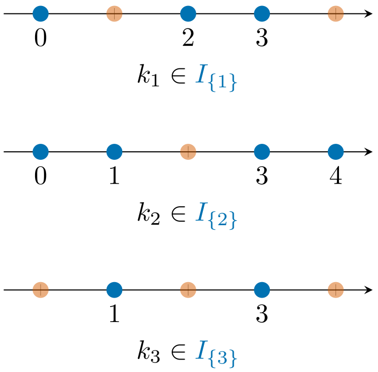


Figure: The one-dimensional index sets $I_{\{j\}}$.



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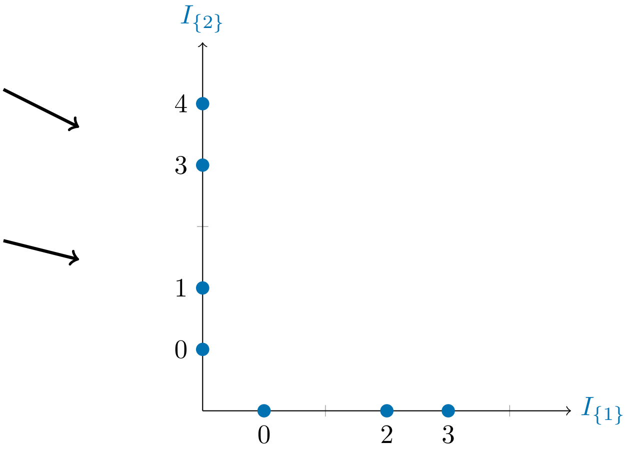
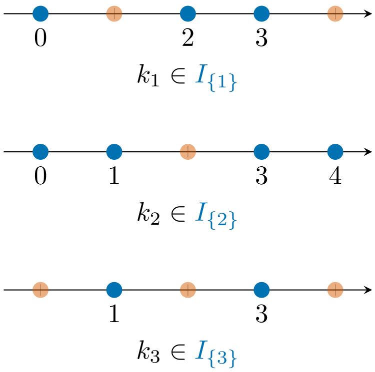


Figure: The two-dimensional candidate set $I_{\{1\}} \times I_{\{2\}}$.



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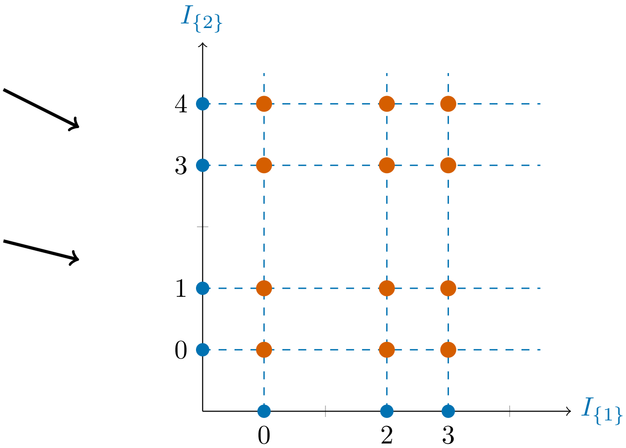

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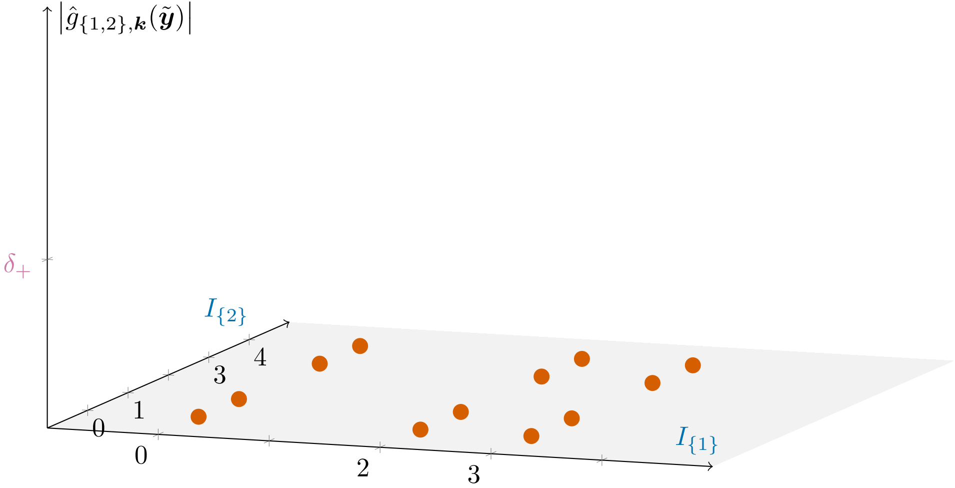

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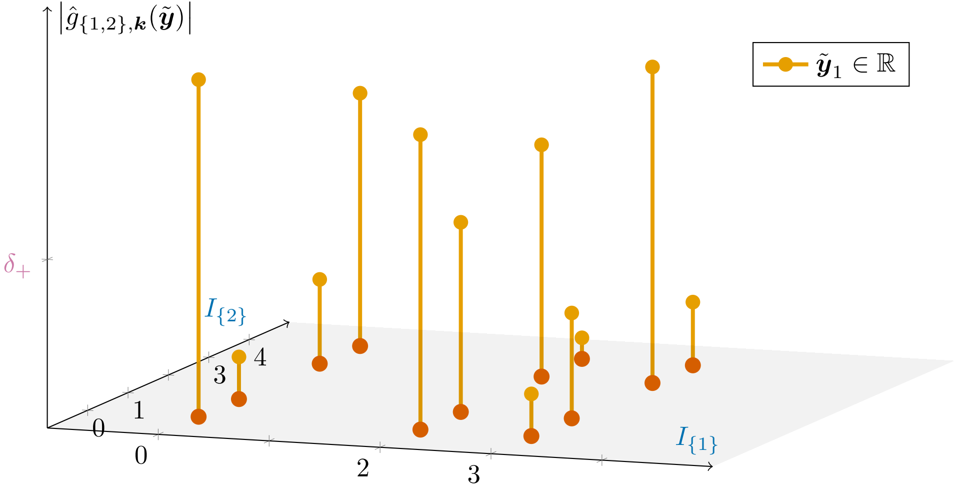

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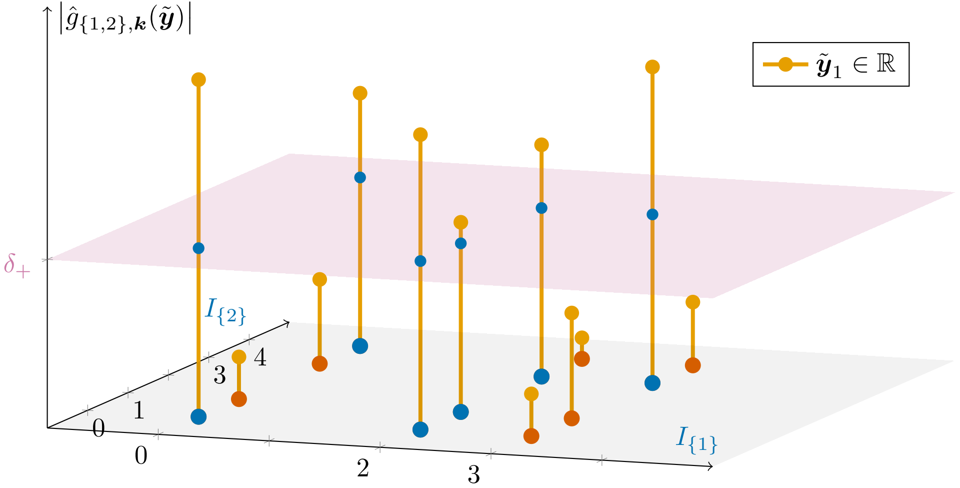

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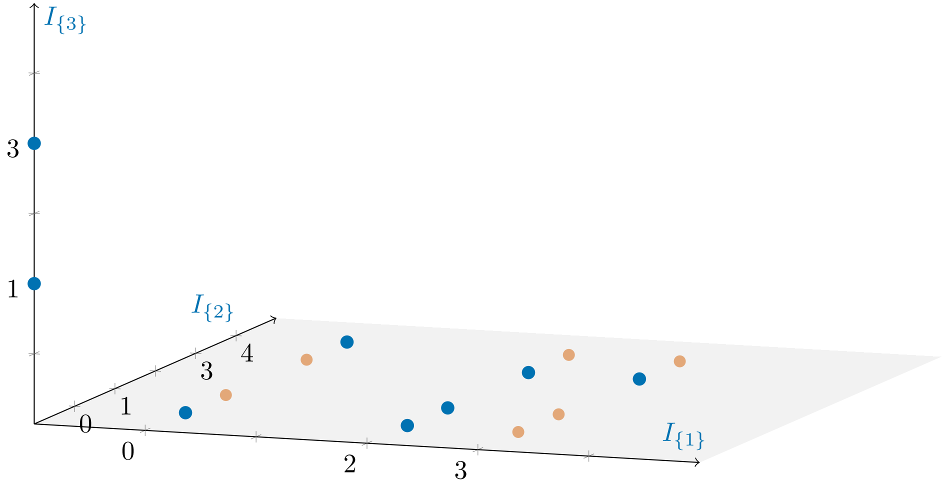

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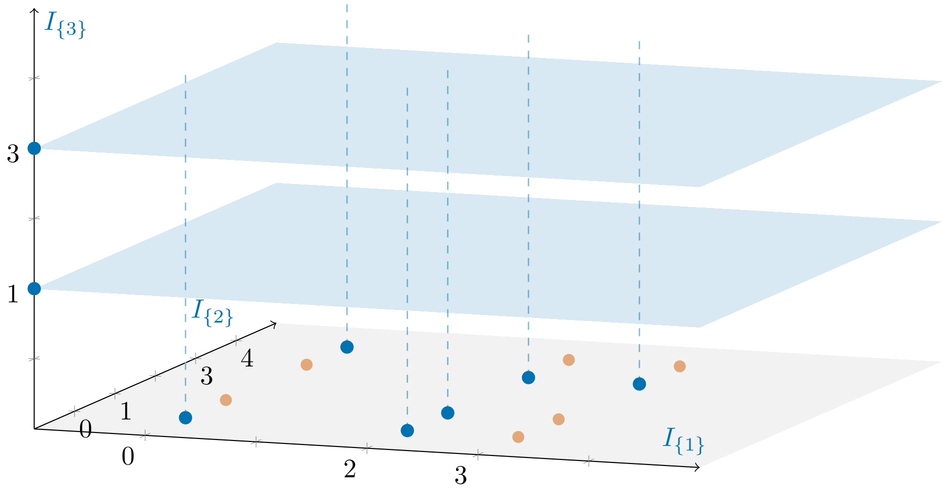

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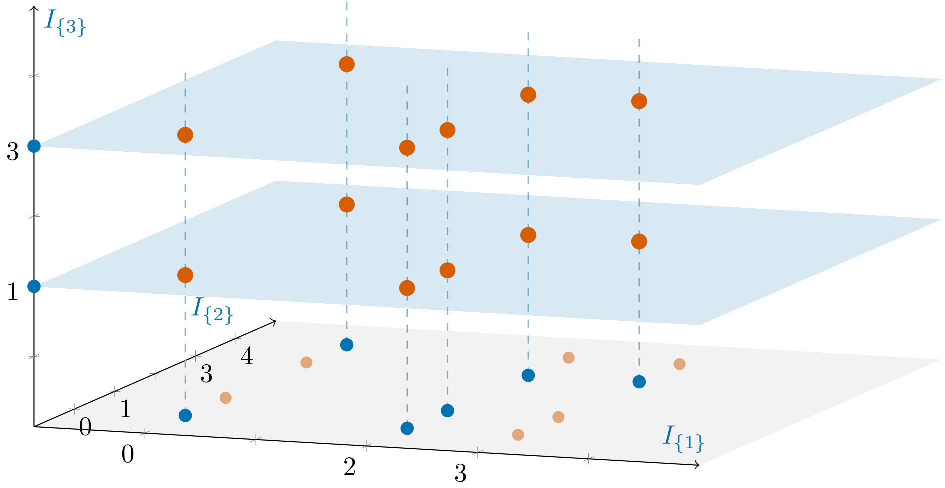

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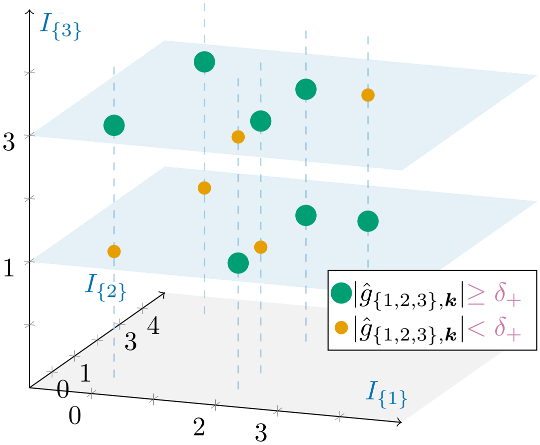

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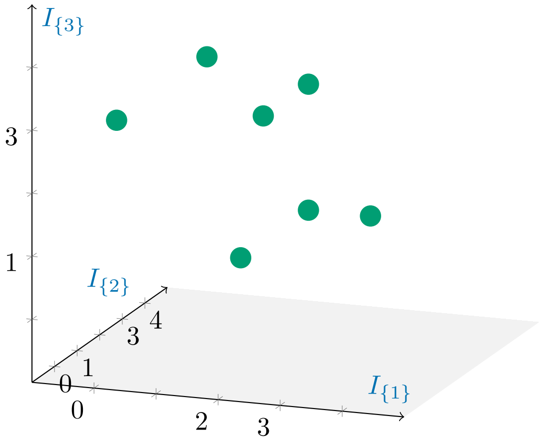

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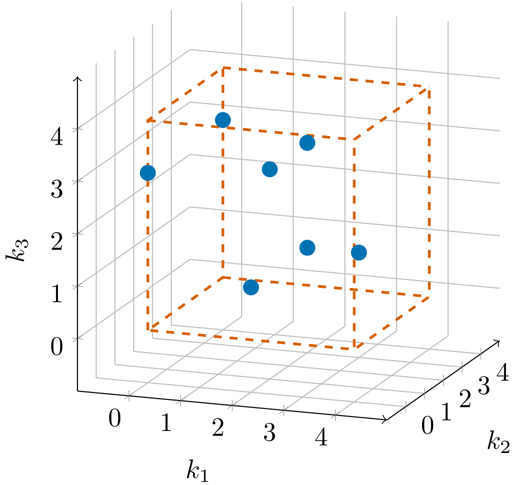

Figure: The correctly detected index set $I = I_{\{1,2,3\}}$.

Poisson equation (one-dimensional)

$$-\frac{d^2}{dx^2}u(x) = f(x), \qquad x \in (0,1)$$
$$u(0) = u(1) = 0$$

- aim: learn $G(f) = u$
- sampling: directly via the analytical solution

Parametrization of f

- one-dimensional Fourier partial sum:

$$f(x) \approx \sum_{\ell=-4}^{4} a_\ell \mathrm{e}^{2\pi \mathrm{i} \ell x}$$

- $n = 9$ Fourier coefficients $\implies$ overall dimension $d + n = 1 + 9 = 10$

Analytical solution

$$u(x, \boldsymbol{a}) = \frac{a_0}{2} x(1-x) + \sum_{\substack{\ell=-4 \\ \ell \neq 0}}^{4} \frac{a_\ell}{4\pi^2 \ell^2} (\mathrm{e}^{2\pi \mathrm{i} \ell x} - 1) \qquad x \in [0,1],\ \boldsymbol{a} \in \mathbb{C}^9$$

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Transformation to $[-1,1]^{10}$

- shift/scale: $x = \frac{1}{2}(\tilde{x}+1)$
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- sparsity $s = 1000$
  search space $\Gamma = [0, 64]^{10}$
- testing with 10^4 randomly drawn $\boldsymbol{a}$
- relative ℓ_2 error evaluated on 1000 equidistant points

Transformed solution

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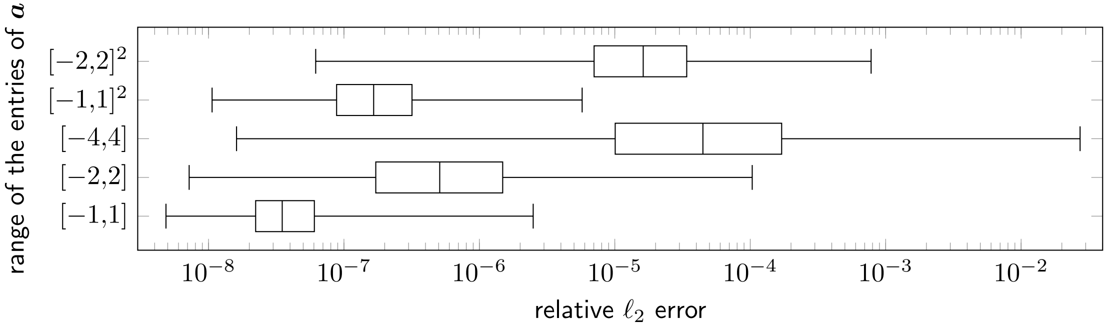

- sparsity $s = 1000$
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- highly structured index set I

Transformed solution

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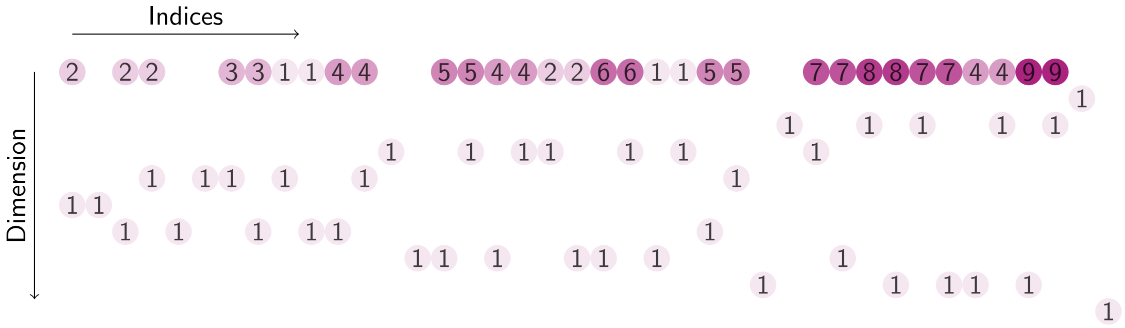

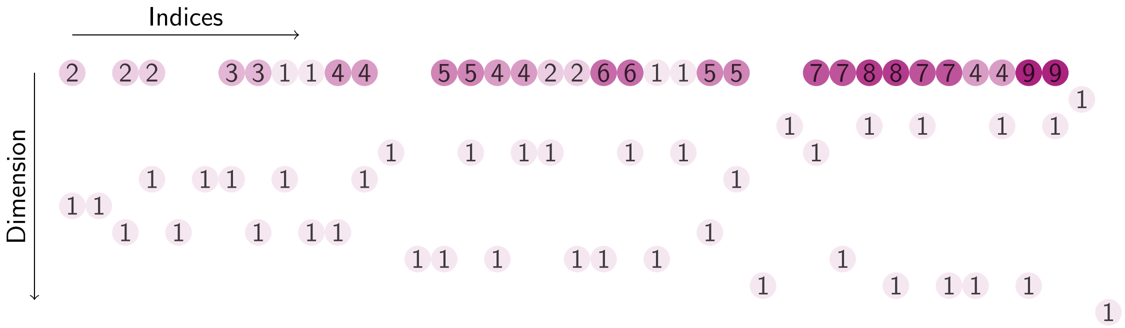

Generalisation to higher dimensions

- learned structure can be generalized to higher dimensions for better resolutions of f, e.g., $n \approx 100$
- same approximation problem, but index set I is no longer unknown
- coefficients $\hat{u}_{\boldsymbol{k}}$ can be computed directly using a QMC method, e.g., rank-1 lattices

Heat equation (one-dimensional)

$$\begin{aligned} \partial_t u &= \frac{1}{16}\partial_{xx} u, & x,t &\in (0,1) \\ u(x,0) &= f(x), & x &\in (0,1) \\ u(0,t) = u(L,t), &= 0 & t &\in (0,1) \end{aligned}$$

- sampling: solve for given f with method of lines based solver

Parametrization of f

- sine series:

$$f(x) \approx \sum_{\ell=1}^{9} a_\ell \sin(\ell \pi x)$$

- restricting $a_\ell \in [-1, 1]$

Exact solution

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- sparsity $s = 1000$
  search space $\Gamma = [0, 64]^{11}$
- relative ℓ_2 approximation error: $\approx 2 \cdot 10^{-3}$
- highly structured index set I:

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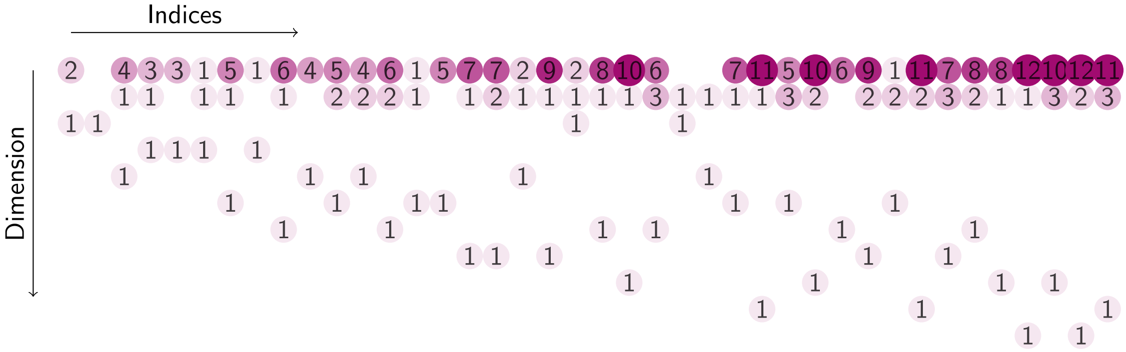

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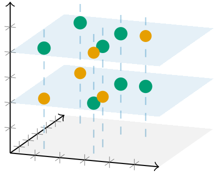

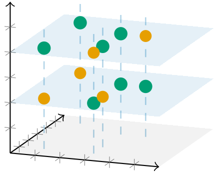

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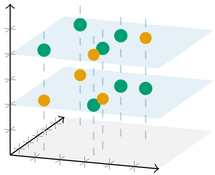

- What did we see?
  - reasonable numerical results and approximation errors
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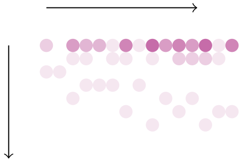
  - results being consistent with analytical solutions for toy examples
- Open problems?
  - Application of our method to more difficult differential problems?
  - Efficient reconstruction methods for our method in various bases?



- Daniel Potts, Fabian Taubert
  Operator learning based on sparse high-dimensional approximation
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Thank you for your attention!

Questions? Ideas? Suggestions?