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# Kernel interpolation on sparse grids

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## **Outline**

- 1. Problem statement**
- 2. Sparse grid approximation**
- 3. Samplet kernel matrix compression**
- 4. Numerical results**



## Setting

- Consider the tensor product Hilbert space

$$\mathcal{H} = \bigotimes_{i=1}^m \mathcal{H}^{(i)}.$$

- Each  $\mathcal{H}^{(i)}$  is a reproducing kernel Hilbert space defined on a Lipschitz region  $\Omega_i \subset \mathbb{R}^{d_i}$  of dimension  $d_i \in \mathbb{N}$ .
- The corresponding reproducing kernels are denoted by  $\kappa_i$ ,  $i = 1, \dots, m$ .
- The space  $\mathcal{H}$  is a reproducing kernel Hilbert space with product kernel

$$\kappa(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^m \kappa_i(x_i, y_i)$$

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- Associated to  $\mathbf{X}$ , we introduce the subspace  $\mathcal{H}_{\mathbf{X}} := \text{span}\{\kappa(\mathbf{x}, \cdot) : \mathbf{x} \in \mathbf{X}\}$ .
- By the reproducing property, the  $\mathcal{H}$ -orthogonal projection  $f_{\mathbf{X}}$  of any  $f \in \mathcal{H}$  onto  $\mathcal{H}_{\mathbf{X}}$  is the interpolant

$$f_{\mathbf{X}}(\mathbf{x}_i) := \sum_{j=1}^{|\mathbf{X}|} \alpha_j \kappa(\mathbf{x}_j, \mathbf{x}_i) = f(\mathbf{x}_i) \quad \text{for all } \mathbf{x}_i \in \mathbf{X}.$$

- Letting  $\mathbf{f} := [f(\mathbf{x}_i)]_i$ , it can be computed by solving the linear system

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## Univariate approximation

- Let  $X_0^{(i)} \subset X_1^{(i)} \subset \dots \subset X^{(i)} \subset \Omega_i$  be a nested sequence of subsets with *fill distance*

$$h_j^{(i)} := \sup_{x \in \Omega_i} \min_{y \in X_j^{(i)}} \|x - y\|_2 \sim 2^{-j}.$$

- Associated to the sequence of points, there is a sequence of subspaces

$$\mathcal{H}_0^{(i)} \subset \mathcal{H}_1^{(i)} \subset \dots \subset \mathcal{H}^{(i)}, \quad \mathcal{H}_j^{(i)} := \text{span} \{ \kappa_i(x, \cdot) : x \in X_j^{(i)} \}.$$

- Assuming  $\mathcal{H}^{(i)} \cong H^{s_i}(\Omega_i)$  for  $s_i > d_i/2$ , there hold the univariate error estimates

$$\|f - P_j^{(i)} f\|_{L^2(\Omega_i)} \lesssim (h_j^{(i)})^{2s_i} \|f\|_{H^{2s_i}(\Omega_i)}, \quad f \in H^{2s_i}(\Omega_i).$$

Herein  $P_j^{(i)} f = f_{X_j^{(i)}}$  denotes the  $\mathcal{H}^{(i)}$ -orthogonal projection onto  $\mathcal{H}_j^{(i)}$ .

- Similarly, the *detail projection*  $Q_j^{(i)} := P_j^{(i)} - P_{j-1}^{(i)}$ ,  $P_{-1}^{(i)} := 0$ , satisfies

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## Sparse grid approximation

■ Based on the detail projections, we introduce the *sparse grid projection*

$$\widehat{\mathbf{P}}_J^w: \mathcal{H} \rightarrow \widehat{\mathcal{H}}_J^w, \quad \widehat{\mathbf{P}}_J^w f = \sum_{j^T w \leq J} (Q_{j_1}^{(1)} \otimes \cdots \otimes Q_{j_m}^{(m)}) f.$$

**Theorem.** Let  $f \in H^{2s}(\Omega)$  and let  $\mathbf{X}$  be quasi-uniform. Denote by  $N := \dim \widehat{\mathcal{H}}_J^w$  the number of degrees of freedom in the sparse tensor product space  $\widehat{\mathcal{H}}_J^w$  and set

$$\beta := 2 \frac{\min\{s_1/w_1, \dots, s_m/w_m\}}{\max\{d_1/w_1, \dots, d_m/w_m\}}.$$

Assume that the minimum in the enumerator is attained  $P \in \mathbb{N}$  times and the maximum in the denominator is attained  $R \in \mathbb{N}$  times. Then, the sparse grid kernel interpolant in  $\widehat{\mathcal{H}}_J^w$  satisfies the error estimate

$$\|(I - \widehat{\mathbf{P}}_J^w)f\|_{L^2(\Omega)} \lesssim N^{-\beta} (\log N)^{(P-1)+\beta(R-1)} \|f\|_{H^{2s}(\Omega)}.$$





## Optimal choice of weights

- For all  $\mathbf{w} > \mathbf{0}$ , there holds

$$\beta \leq \beta^* := 2 \min\{s_1/d_1, \dots, s_m/d_m\}.$$

- Let  $2s_\ell/d_\ell = \beta^*$ . Then the maximum rate  $\beta = \beta^*$  is attained for all  $\mathbf{w} > \mathbf{0}$  such that

$$\frac{s_m}{s_j} \leq \frac{w_\ell}{w_j} \leq \frac{d_\ell}{d_j}, \quad i = 1, 2, \dots, m.$$

- Equilibration of accuracy:** Set  $w_i \sim s_i$  such that

$$2^{-2Js_1/w_1} = 2^{-2Js_2/w_2} = \dots = 2^{-2Js_m/w_m}.$$

- Equilibration of DOFs:** Set  $w_i \sim d_i$  such that

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- Equilibration of cost-benefit rate:** Set  $w_i \sim (d_i + 2s_i)$  such that

$$2^{j_1(d_1+2s_1)} \cdot 2^{j_2(d_2+2s_2)} \dots 2^{j_m(d_m+2s_m)} = 2^{J \cdot \text{const.}}, \quad \mathbf{j}^T \mathbf{w} = J.$$



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## Sparse grid combination technique

- Due to the Galerkin orthogonality, the detail projections satisfy

$$(\mathbf{Q}_j u, \mathbf{Q}_{j'} v)_{\mathcal{H}} = 0 \quad \text{for } j \neq j' \text{ and any } u, v \in \mathcal{H},$$

as a consequence, the sparse grid combination technique is exact.

- We introduce the tensor product projector  $\mathbf{P}_j := \sum_{\ell \leq j} \mathbf{Q}_\ell$  and define the *combination technique index set*  $\mathcal{J}^w := \{j \in \mathbb{N}_0^m : J - |w| < j^T w \leq J\}.$

- There holds

$$\hat{\mathbf{P}}_J^w f = \sum_{j \in \mathcal{J}^w} c_j^w \mathbf{P}_j f, \quad \text{where } c_j^w := \sum_{\substack{j' \in \{0,1\}^m \\ (j+j')^T w \leq J}} (-1)^{|j'|}.$$

- As a consequence, we only need to solve the smaller tensor product problems

$$\mathbf{K}_j \alpha_j := (\mathbf{K}_{j_1}^{(1)} \otimes \cdots \otimes \mathbf{K}_{j_m}^{(m)}) \alpha_j = f_j.$$



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$$\mathbf{K}_j \alpha_j := (\mathbf{K}_{j_1}^{(1)} \otimes \cdots \otimes \mathbf{K}_{j_m}^{(m)}) \alpha_j = f_j.$$





## Sparse grid combination technique

- Due to the Galerkin orthogonality, the detail projections satisfy

$$(\mathbf{Q}_j u, \mathbf{Q}_{j'} v)_{\mathcal{H}} = 0 \quad \text{for } j \neq j' \text{ and any } u, v \in \mathcal{H},$$

as a consequence, the sparse grid combination technique is exact.

- We introduce the tensor product projector  $\mathbf{P}_j := \sum_{\ell \leq j} \mathbf{Q}_\ell$  and define the *combination technique index set*  $\mathcal{J}^{\mathbf{w}} := \{j \in \mathbb{N}_0^m : J - |\mathbf{w}| < j^T \mathbf{w} \leq J\}$ .

- There holds

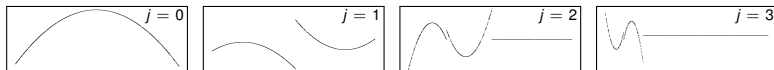
$$\widehat{\mathbf{P}}_J^{\mathbf{w}} f = \sum_{j \in \mathcal{J}^{\mathbf{w}}} c_j^{\mathbf{w}} \mathbf{P}_j f, \quad \text{where } c_j^{\mathbf{w}} := \sum_{\substack{j' \in \{0,1\}^m \\ (j+j')^T \mathbf{w} \leq J}} (-1)^{|j'|}.$$

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## Samplelets



- Let  $\mathcal{X}'_0 \subset \mathcal{X}'_1 \subset \dots \subset \mathcal{X}'_j := \mathcal{X}' := \text{span}\{\delta_x : x \in X\}$ .
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$$(\sigma_{j,k}, p)_\Omega = 0 \quad \text{for all } p \in \mathcal{P}_q(\Omega).$$

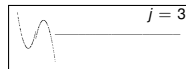
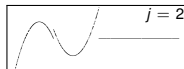
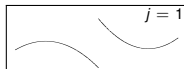
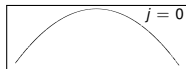
- Since  $\mathcal{X}'_j \subset \mathcal{H}'$ , samplelets induce a multiresolution basis for  $\mathcal{H}_X$  via the embedding

$$\sigma_{j,k} = \sum_{\ell} u_{j,k,\ell} \delta_{x_\ell} \mapsto \psi_{j,k} = \sum_{\ell} u_{j,k,\ell} \kappa(x_\ell, \cdot).$$

- There holds  $[\langle \psi_{j,k}, \psi_{j',k'} \rangle_{\mathcal{H}}]_{j,j',k,k'} = \mathbf{TKT}^\top$ .



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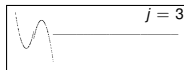
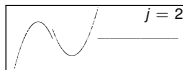
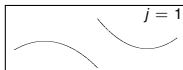
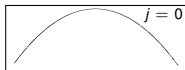
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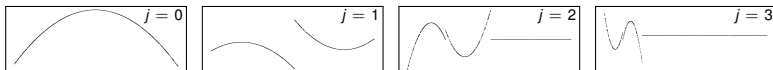
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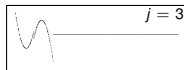
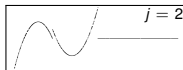
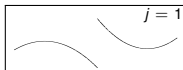
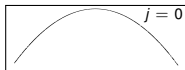
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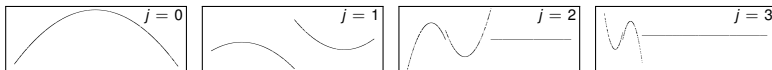
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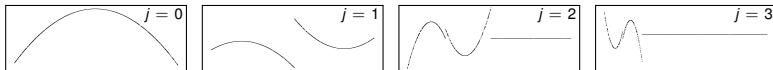
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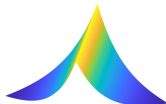
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## Sample kernel matrix compression

- For the compression of kernel matrices we make the *asymptotical smoothness* assumption



$$\frac{\partial^{|\alpha|+|\beta|}}{\partial x^\alpha \partial y^\beta} \kappa(x, y) \leq c_K \frac{(|\alpha| + |\beta|)!}{\rho^{|\alpha|+|\beta|} \|x - y\|_2^{|\alpha|+|\beta|}}, \quad c_K, \rho > 0.$$

**Theorem.** Let the data set  $X$  be quasi-uniform. Then, setting all coefficients of the transformed kernel matrix  $\mathbf{K}^\Sigma := \mathbf{T} \mathbf{K} \mathbf{T}^\top$  to zero which satisfy

$$\text{dist}(\tau, \tau') \geq \eta \max\{\text{diam}(\tau), \text{diam}(\tau')\}, \quad \eta > 0,$$

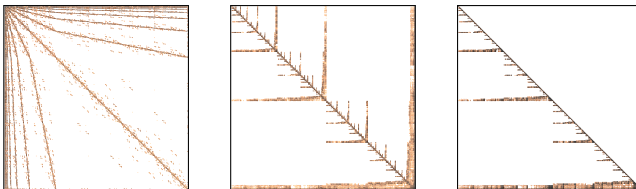
results in a consistency error of

$$\frac{\|\mathbf{K}^\Sigma - \mathbf{K}_\eta^\Sigma\|_F}{\|\mathbf{K}^\Sigma\|_F} \lesssim (\eta \rho / d)^{-2(q+1)}.$$

The compressed matrix  $\mathbf{K}_\eta^\Sigma$  only contains  $\mathcal{O}(|X| \log |X|)$  entries.



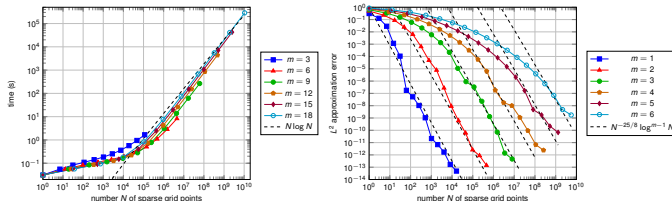
## Sparse direct solver



- The samplelet compression yields an essentially sparse matrix.
- Corresponding linear systems can be solved by first performing a fill-in reducing reordering (nested dissection) and the Cholesky factorization.
- In the numerical examples, we employ CHOLMOD.



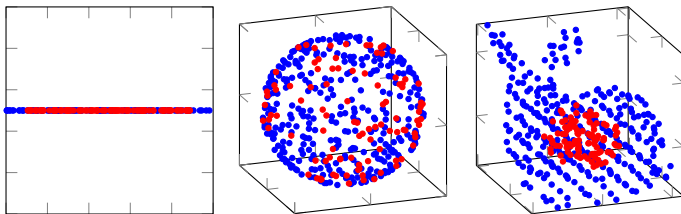
## Benchmark in $(0, 1)^m$



- In each direction, we consider the Matérn-17/16 kernel and set  $f = 1$ .
- The energy space is  $H^{25/16}(0, 1)$  and the expected rate of convergence is  $25/8$ .
- We use equidistant points  $X_j = \{2^{-(j+1)}k : k = 1, 2, \dots, 2^{j+1} - 1\}$ .
- The error is computed using a 4-point Gaussian quadrature rule in each direction.



## Tensor product of 1 + 2 + 3 dimensional regions

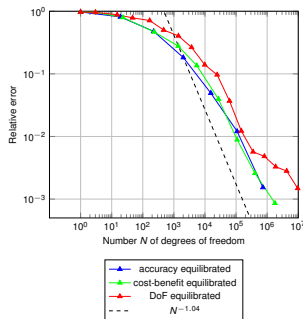


- On  $[0, 1]$  and  $\mathbb{S}^2$ , we create nested point sets from uniform random points.
- For the Stanford bunny nested point sets are created from a volume mesh.
- We consider the Matérn- $\left(\frac{25}{16} - \frac{d}{2}\right)$  kernel,  $d = 1, 2, 3$ .
- The energy space is  $H^{25/16}(\Omega_i)$  and the expected rate of convergence is  $25/8$ .
- The interpolation error is evaluated at 100 random points in each region.



## Convergence

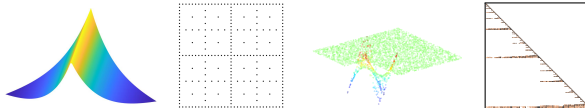
	Interval		Sphere		Rabbit	
	$qx_i$	$hx_i, x_j$	$qx_i$	$hx_i, x_j$	$qx_i$	$hx_i, x_j$
$j = 0$	—	$6.80 \cdot 10^{-1}$	—	2.00	—	1.01
$j = 1$	$6.25 \cdot 10^{-2}$	$4.45 \cdot 10^{-1}$	$4.03 \cdot 10^{-1}$	1.24	$1.01 \cdot 10^{-1}$	$5.82 \cdot 10^{-1}$
$j = 2$	$2.34 \cdot 10^{-2}$	$2.03 \cdot 10^{-1}$	$5.49 \cdot 10^{-2}$	$5.66 \cdot 10^{-1}$	$3.57 \cdot 10^{-2}$	$3.01 \cdot 10^{-1}$
$j = 3$	$7.81 \cdot 10^{-3}$	$1.41 \cdot 10^{-1}$	$1.62 \cdot 10^{-2}$	$2.87 \cdot 10^{-1}$	$1.28 \cdot 10^{-2}$	$1.76 \cdot 10^{-1}$
$j = 4$	$7.81 \cdot 10^{-3}$	$1.33 \cdot 10^{-1}$	$7.01 \cdot 10^{-4}$	$1.62 \cdot 10^{-1}$	$8.12 \cdot 10^{-3}$	$1.06 \cdot 10^{-1}$
$j = 5$	$7.81 \cdot 10^{-3}$	$4.68 \cdot 10^{-2}$	$6.48 \cdot 10^{-4}$	$8.22 \cdot 10^{-2}$	$3.63 \cdot 10^{-3}$	$4.69 \cdot 10^{-2}$
$j = 6$	$7.81 \cdot 10^{-3}$	$7.81 \cdot 10^{-3}$	$4.22 \cdot 10^{-5}$	$2.92 \cdot 10^{-2}$	$1.99 \cdot 10^{-3}$	$1.83 \cdot 10^{-2}$



- The fill distance approximately halves from one level to another.
- We (almost) observe the expected rate  $\beta = 25/24 \approx 1.04$  for all choices of weights.



## Conclusion



- We have extended existing approximation results to kernel interpolation on sparse grids, including super convergence.
- In the considered setting, the sparse grid combination technique is exact and can be used for computations.
- The resulting smaller tensor product problems have been solved in sample coordinates using a sparse direct solver.
- The numerical results in  $1 + 2 + 3$  dimensions confirm the theoretical rates for general data sets.



# Thank you

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