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### DTU Compute Department of Applied Mathematics and Computer Science





# Adaptive spectral tensor-train decomposition for the construction of surrogate models

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**PyPI**: https://pypi.python.org/pypi/TensorToolbox/ (LGPLv3) **^**: http://www2.compute.dtu.dk/~dabi/

### Introduction

The construction of surrogate models is important as a mean of acceleration in computational methods for uncertainty quantification (UQ). When the forward model is particularly expensive, surrogate models can be used for the forward propagation of uncertainty [4] and the solution of inference problems [5]. An adaptive



0.8

1.0 0.0

corner peak - d=20

construction is necessary to meet the prescribed accuracy tolerances with the lowest computational effort.

### **Problem setting**

We consider  $f \in L^2_{\mu}([a, b]^d)$ ,  $d \gg 1$ , and  $\mathbf{x} \in [a, b]^d$ to be the variables entering the formulation of a parametric problem.

When to construct a surrogate?

- f is computationally expensive
- f needs to be evaluated many times
- the construction complexity pays off

## **Spectral tensor-train**

**Functional tensor-train approximation [1]** For  $\mathbf{r} = (1, r_1, \dots, r_{d-1}, 1)$ , let  $f_{TT}$  be s.t.  $f_{TT} = \arg \min \|f - g\|_{L^2_{\mu}}$  $g \in L^2_{\mu}$  $g(\mathbf{x}) = \sum \gamma_1(\alpha_0, x_1, \alpha_1) \cdots \gamma_d(\alpha_{d-1}, x_d, \alpha_d)$  $\alpha_0, \ldots, \alpha_d = 1$ 

where  $\langle \gamma_k(i,\cdot,m), \gamma_k(i,\cdot,n) \rangle_{L^2_{\mu}} = \delta_{mn}$ .

**FTT-approximation convergence** [1]

### **Anisotropic adaptivity**



For 
$$f \in \mathcal{H}^k_{\mu}$$
,  $k > d - 1$  and  $R_{TT} = f - f_{TT}$ ,  
$$\lim_{r \to \infty} \|R_{TT}\|_{L^2_{\mu}} = 0$$

#### **FTT-decomposition and Sobolev spaces** [1]

Let  $\mathbf{I} \subset \mathbb{R}^d$  be closed and bounded, and  $f \in \mathcal{I}$  $L^2_{\mu}(\mathbf{I})$  be a Hölder continuous function with exponent > 1/2 such that  $f \in \mathcal{H}^k_{\mu}(\mathbf{I})$ . Then  $f_{TT}$  is such that  $\gamma_j(\alpha_{j-1}, \cdot, \alpha_j) \in \mathcal{H}^k_{\mu_j}(I_j)$  for all  $j, \alpha_{j-1}$ and  $\alpha_i$ .

Let  $P_{\mathbf{N}} : L^2_{\mu}(\mathbf{I}) \to \operatorname{span}\left(\left\{\Phi_{\mathbf{i}}\right\}_{\mathbf{i}=0}^{\mathbf{N}}\right)$  where  $\left\{\Phi_{\mathbf{i}}\right\}_{\mathbf{i}=0}^{\mathbf{N}}$ are orthogonal polynomials:

#### **STT-Projection**

$$P_{\mathbf{N}}f_{TT} = \sum_{\mathbf{i}=0}^{\mathbf{N}} c_{\mathbf{i}}\Phi_{\mathbf{i}}$$
$$c_{\mathbf{i}} = \sum_{\alpha_{0},\dots,\alpha_{d}=1}^{\mathbf{r}} \beta_{1}(\alpha_{0}, i_{1}, \alpha_{1})\dots\beta_{d}(\alpha_{d-1}, i_{d}, \alpha_{d})$$
$$\beta_{n}(\alpha_{n-1}, i_{n}, \alpha_{n}) = \int_{I_{n}} \gamma_{n}(\alpha_{n-1}, x_{n}, \alpha_{n})\phi_{i_{n}}(x_{n})\mu_{n}(dx_{n})$$

Oscillatory: 
$$f_1(\mathbf{x}) = \cos\left(\sum_{i=1}^d 2^{c_i} x_i\right)$$
  
Corner Peak:  $f_2(\mathbf{x}) = \left(1 + \sum_{i=1}^d 2^{c_i} x_i\right)^{-(d+1)}$   
 $c_i \sim \begin{cases} Be(2,8) & \text{if } p_i < 0.5\\ Be(8,2) & \text{otherwise} \end{cases}$   
 $p_i \sim \text{Bernoulli}(0.5)$ 

The performances are evaluated on the Genz functions up to d = 100, and compared to the results obtained with the anisotropic Smolyak pseudo-spectral approximation [2]. The adaptivity avoids over-fitting and under-fitting due to discrepancy between the polynomial order and the FTT tolerance.

#### Uncertain wave loads on offshore monopiles





### Features

- Linear scaling w.r.t. d
- Incremental construction
- Storage and re-starting
- Parallel implementation

## **STT-Projection convergence** Let $f \in \mathcal{H}^k_{\mu}(\mathbf{I})$ , then $\|f - P_N f_{TT}\|_{L^2_{\mu}} \le D(k) r^{-\frac{k+1-d}{2}} \|f\|_{\mathcal{H}^k_{\mu}}$ $+ C(k)N^{-k}|f_{TT}|_{\mu,k}$

The construction is performed using the tensor-train decomposition [6] of tensorized quadrature rules, obtained through the deterministic sampling algorithm TT-dmrg-cross [7], achieving scalable  $\mathcal{O}(dNr^2)$  complexity.

#### $5 \times 10^{-1}$ $1 \times 10^{-1}$ | 236 | $2.4 \times 10^{-2}$ | 9.866 × 10<sup>-2</sup> N $5 \times 10^{-2}$ 260 $7.3 \times 10^{-3}$ 9.766 $\times 10^{-2}$ N x [m]

 Investigation of nested rules • UQ on 3D water waves [3] interaction with structures

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