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

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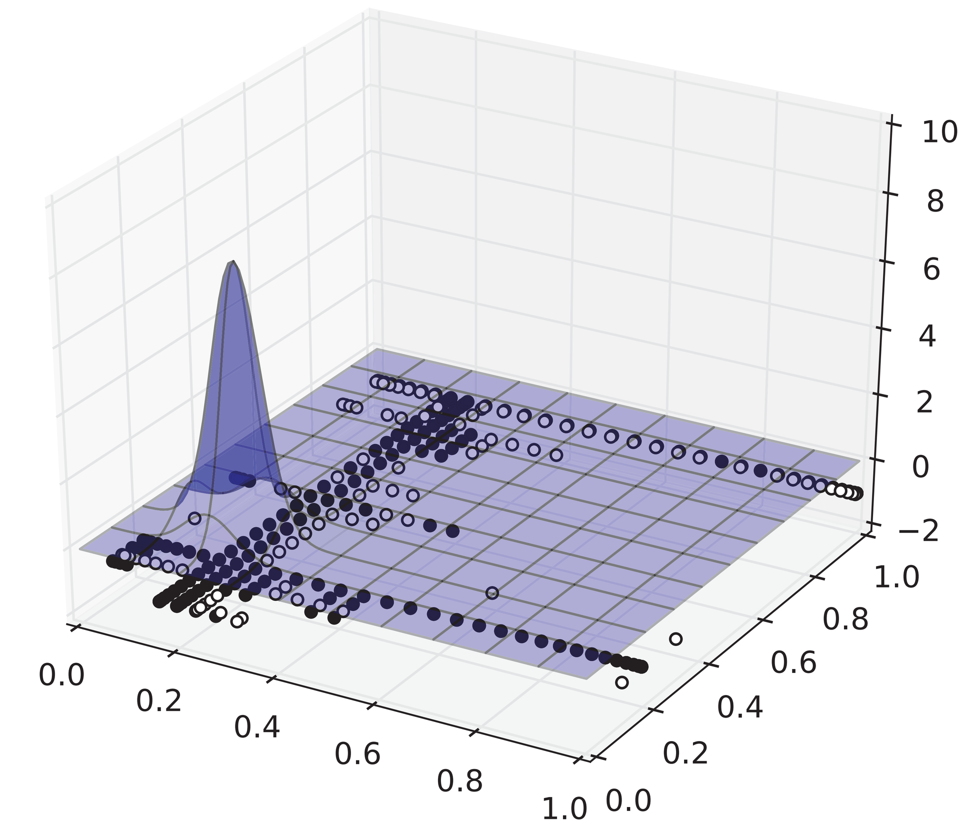
PyPI: https://pypi.python.org/pypi/TensorToolbox/ (LGPLv3)
: http://www2.compute.dtu.dk/~dabi/



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 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.

$$f_{TT} = \arg\min_{g \in L^2_\mu} \| f - g \|_{L^2_\mu}$$

$$g(\mathbf{x}) = \sum_{\alpha_0,\dots,\alpha_d=1}^{\mathbf{r}} \gamma_1(\alpha_0, x_1, \alpha_1) \cdots \gamma_d(\alpha_{d-1}, x_d, \alpha_d)$$

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

FTT-approximation convergence [1]

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 $f \in L^2_\mu(\mathbf{I})$ 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, α_{j-1} and α_j.

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

STT-Projection

$$P_\mathbf{N} f_{TT} = \sum_{\mathbf{i}=0}^{\mathbf{N}} c_\mathbf{i} \Phi_\mathbf{i}$$

$$c_\mathbf{i} = \sum_{\alpha_0,\dots,\alpha_d=1}^{\mathbf{r}} \beta_1(\alpha_0, i_1, \alpha_1) \dots \beta_d(\alpha_{d-1}, i_d, \alpha_d)$$

$$\beta_n(\alpha_{n-1}, i_n, \alpha_n) = \int_{I_n} \gamma_n(\alpha_{n-1}, x_n, \alpha_n) \phi_{i_n}(x_n) \mu_n(dx_n)$$

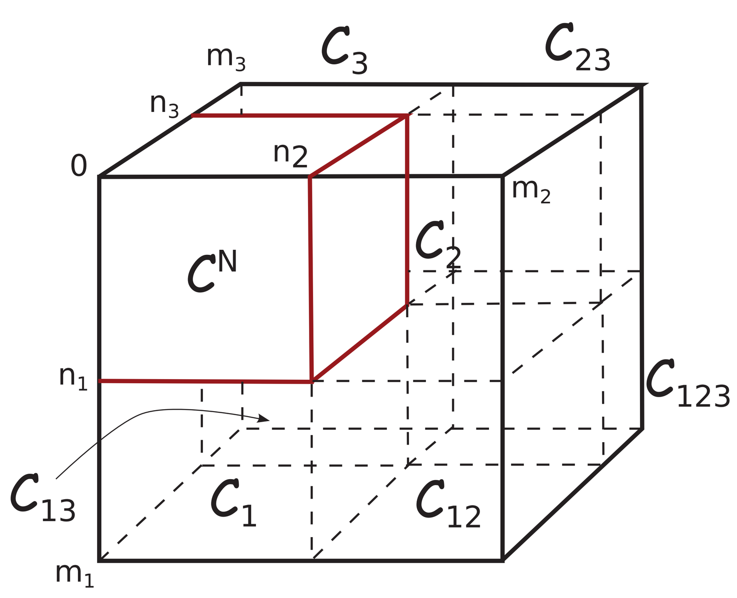
STT-Projection convergence

Let $f \in \mathcal{H}^k_\mu(\mathbf{I})$, then

$$\| f - P_N f_{TT} \|_{L^2_\mu} \leq D(k) r^{-\frac{k+1-d}{2}} \| f \|_{\mathcal{H}^k_\mu} + C(k) N^{-k} | f_{TT} |_{\mu,k}$$

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.

Anisotropic adaptivity

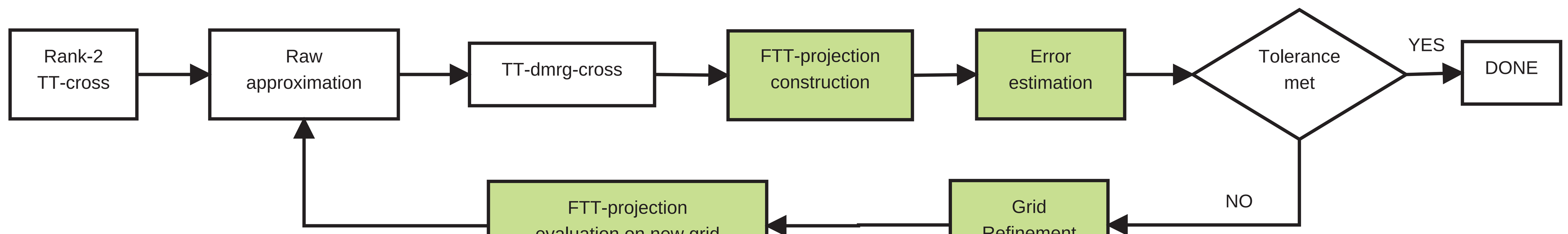


Let $\mathbf{N} = (n_1, \dots, n_{d_s})$ and $\mathbf{M} = (m_1, \dots, m_{d_s})$ s.t. $\mathbf{N} < \mathbf{M}$. Then

$$\| P_\mathbf{N} f_{TT} - P_\mathbf{M} f_{TT} \|_{L^2_\mu} = \sqrt{\sum_{\mathbf{i}=\mathbf{N}}^{\mathbf{M}} c_\mathbf{i}^2} = \sqrt{\sum_{\#\mathbf{i}=1} \|\mathcal{C}_\mathbf{i}\|_F^2 + \sum_{\#\mathbf{i}=2} \|\mathcal{C}_\mathbf{i}\|_F^2 + \cdots}$$

Let us define the n-th order error contribution in the j-th direction:

$$\mathscr{E}_j^{(n)} = \left(\|\mathcal{C}_j\|_F^2 + \sum_{\substack{\#\mathbf{i}=2 \\ j \in \mathbf{i}}} \|\mathcal{C}_\mathbf{i}\|_F^2 + \cdots + \sum_{\substack{\#\mathbf{i}=n \\ j \in \mathbf{i}}} \|\mathcal{C}_\mathbf{i}\|_F^2 \right)^{\frac{1}{2}}$$



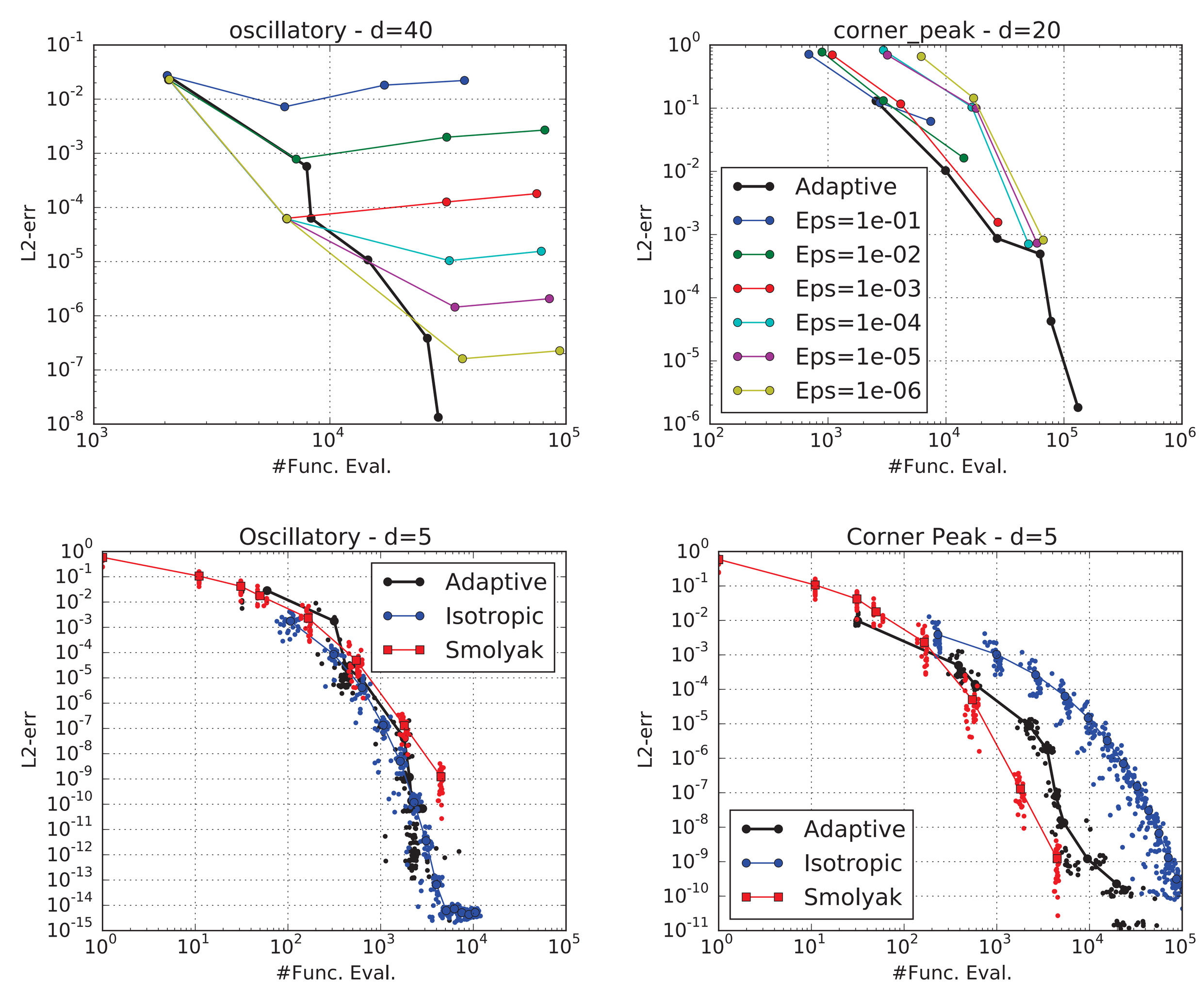
Numerical experiments – Modified Genz functions

Oscillatory : $f_1(\mathbf{x}) = \cos\left(\sum_{i=1}^{d} 2^{c_i} x_i \right)$

Corner Peak : $f_2(\mathbf{x}) = \left(1 + \sum_{i=1}^{d} 2^{c_i} x_i \right)^{-(d+1)}$

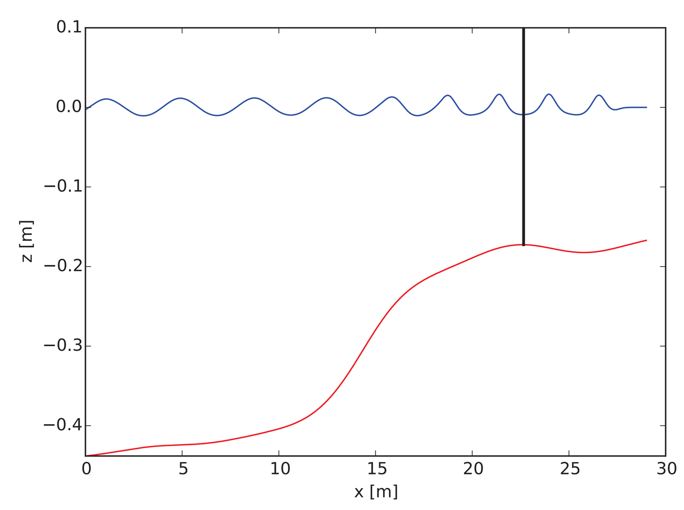
$$c_i \sim \begin{cases} Be(2,8) & \text{if } p_i < 0.5 \\ Be(8,2) & \text{otherwise} \end{cases}$$

$p_i \sim \mathrm{Bernoulli}(0.5)$



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



Scalable flexible-order finite difference of nonlinear and dispersive potential flow [3] for shoaling water waves subject to uncertain bathymetry ($d = 10$).

ε	N.f.e.	L^2-err	E[Load]
5×10^{-1}	221	3.8×10^{-2}	9.962×10^{-2} N
1×10^{-1}	236	2.4×10^{-2}	9.866×10^{-2} N
5×10^{-2}	260	7.3×10^{-3}	9.766×10^{-2} N

Features

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

Outlook

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

References

[1] Bigoni, D., Engsig-Karup, A. P., and Marzouk, Y. M. Spectral tensor-train decomposition. http://arxiv.org/abs/1405.5713.

[2] Conrad, P., and Marzouk, Y. Adaptive Smolyak pseudospectral approximations. *SIAM Journal on Scientific Computing* (2013).

[3] Engsig-karup, A. P., Glimberg, S. L., and Nielsen, A. S. Fast hydrodynamics on heterogeneous many-core hardware. In *Designing Scientific Applications on GPUs*, Chapman & Hall/CRC Numerical Analy & Scient Comp. Series. Chapman and Hall/CRC, Nov. 2013, pp. 251–294.

[4] Le Maître, O. P., and Knio, O. M. *Spectral Methods for Uncertainty Quantification.* Scientific Computation. Springer Netherlands, Dordrecht, June 2010.

[5] Marzouk, Y. M., and Najm, H. N. Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems. *Journal of Computational Physics 228*, 6 (Apr. 2009), 1862–1902.

[6] Oseledets, I. Tensor-train decomposition. *SIAM Journal on Scientific Computing 33*, 5 (2011), 2295–2317.

[7] Savostyanov, D., and Oseledets, I. Fast adaptive interpolation of multi-dimensional arrays in tensor train format. *The 2011 International Workshop on Multidimensional (nD) Systems* (Sept. 2011), 1–8.