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Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Adaptive spectral tensor-train decomposition for the construction of surrogate models

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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 $f \in L^2([a,b]^d)$, $d \gg 1$, and $x \in [a,b]^d$ 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 $r = (r_1, r_2, \ldots, r_d)$, let $f_{rT}$ be s.t.

$$f_{rT} = \arg \min_{f \in L^2} \| f - \varrho \|_{L^2}$$

$$g(x) = \sum_{\alpha_1, \ldots, \alpha_d = 1} \gamma(\alpha_1 x_1, \alpha_2) \cdots \gamma(\alpha_d x_d, \alpha_d)$$

where $(\gamma(i; m), \gamma(i; n)) = \delta_{mn}$.

FTT-approximation convergence [1]
For $f \in H^s_k$, $k > d - 1$ and $RTT = f - f_{rT}$,

$$\lim_{r \to \infty} \| RTT \|_{L^2} = 0$$

FTT-decomposition and Sobolev spaces [1]
Let $I \subset [a,b]$ be closed and bounded, and $f \in L^2(I)$ be a Hölder continuous function with exponent $> 1/2$ such that $f \in H^{s_k}(I)$. Then $f_{rT}$ is such that $\gamma(\alpha_1, \ldots, \alpha_d) \in H^{s_k}(I)$ for all $\alpha_1, \ldots, \alpha_d$.

Let $P_k : L^2(I) \to \text{span} \{ \phi_i \}_{i=1}^N$ where $\{ \phi_i \}_{i=1}^N$ are orthogonal polynomials:

STT-projection

$$P_k (f) = \sum_{i=1}^N \phi_i \langle \phi_i, f \rangle$$

$$\alpha = \sum_{\alpha_1, \ldots, \alpha_d = 1} \beta(\alpha_1, \ldots, \alpha_d)$$

$$\beta(\alpha_1, \ldots, \alpha_d) = \int_I \gamma(\alpha_1 x_1, \ldots, \alpha_d x_d) \phi_i(x) \, dx$$

STT-projection convergence

Let $f \in H^{s_k}(I)$, then

$$\| f - P_k f \|_{L^2} \leq D(k) \| f \|_{H^{s_k}}$$

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

Anisotropic adaptivity

Let $N = (n_1, \ldots, n_d)$ and $M = (m_1, \ldots, m_d)$ s.t. $N < M$. Then

$$\| P_{k_{TT}} f - P_{M_{TT}} f \|_{L^2} \leq \sum_{i=1}^M | c_i | \| f \|_{H^{s_k}} \cdots$$

Smoothed functions

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

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

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.

Numerical experiments – Modified Genz functions

Uncertain wave loads on offshore monopiles

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

References

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