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

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Abstract

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 and the solution of inference problems. An adaptive construction is necessary to meet the prescribed accuracy tolerances with the lowest computational effort.

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 a function $f$ to be the variables entering the formulation of a parametric problem.

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

Spectral tensor-train

Functional tensor-train approximation

For $r = (r_1, r_2, \ldots, r_{d-1})$, let $f_{TT}^r$ be s.t.

$$f_{TT} = \arg \min_{g \in \mathcal{P}_{d1}} \| f - g \|_{L_2^d}$$

where $g(x) = \sum_{\alpha_1, \ldots, \alpha_d} \gamma(\alpha_1, x_1, \alpha_d) \cdot \cdots \cdot \gamma(\alpha_{d-1}, x_{d-1}, \alpha_2)$

TT-decomposition and Sobolev spaces

Let $I \subset \mathbb{R}^d$ be closed and bounded, and $f \in L_2^d(I)$ be a Hölder continuous function with exponent $> 1/2$ such that $f \in H^s(I)$. Then $f_{TT}$ is such that $\gamma(\alpha_1, \ldots, \alpha_d) \in H^s(I)$ for all $\alpha_1, \ldots, \alpha_d$.

Let $P_k : L_2^d(I) \rightarrow \text{span} \{ \phi_i \}_{i=1}^N$ where $\{\phi_i\}_{i=1}^N$ are orthogonal polynomials:

- STT-Projection

$$P_k f_{TT} - \sum_{i=1}^N c_i \phi_i$$

$$c_i = \int I f(x) \phi_i(x) dx$$

- STT-projection convergence

Let $f \in H^s(I)$, then

$$\| f - P_k f_{TT} \|_{L_2^d} \leq C(k) r^{-s} \| f \|_{L_2^d}$$

The construction is performed using the tensor-train decomposition [8] of tensorized quadrature rules, obtained through the deterministic sampling algorithm TT-darg-cross [7], achieving O(dN^2) complexity.

Numerical experiments – Modified Genz functions

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

Corner Peak: $f(x) = \left( 1 + \sum_{i=1}^d x_i \right)^{10}$

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 FFT tolerance.

Anisotropic adaptivity

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

$$|P_N f_{TT} - P_M f_{TT}|_2 \leq \sum_{i=1}^M c_i \left( \sum_{||\alpha||=0} \| C_{\alpha} \|_{L_2^d} + \cdots + \| C_{\alpha} \|_{L_2^d} \right)^{1/2}$$

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

$$\delta_{j,n} = \left( \| C_{\alpha} \|_{L_2^d} + \cdots + \| C_{\alpha} \|_{L_2^d} \right)^{1/2}$$

Outlook

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

References