MascotNum2020 conference - Principal Component Analysis and boosted optimal weighted least-squares for training tree tensor networks

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Abstract: One of the most challenging tasks in computational science is the approximation of high-dimensional functions. Supervised learning algorithms construct the approximation of a function u using point evaluations of this function. When function's evaluations are costly, only a limited number N of evaluations can be performed. In an active learning setting, the point evaluations can be selected adaptively, which is relevant when no expensive simulations have yet been made.

In this work, we propose a strategy to construct an approximation v of a function u belonging to $L^2_\mu(\mathcal{X})$, the space of square-integrable functions defined on a product set $\mathcal{X} = \mathcal{X}_1 \times \ldots \times \mathcal{X}_d$, equipped with a probability measure μ. The algorithm constructs the approximation v in tree-based tensor format thanks two main ingredients: an extension of principal component analysis (PCA) to multivariate functions [5], and weighted least-squares projections [2, 3]. More precisely, tree-based tensor formats are tree tensor networks whose graphs are dimension partition trees. Low-order tensors v_α, seen as vector-valued maps, are associated to each node α of a dimension partition tree T, and this set of tensors completely parametrizes the approximation.

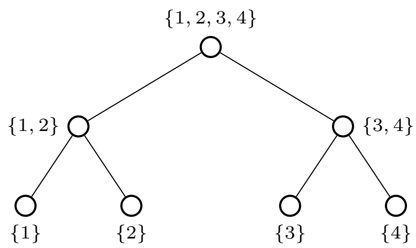

Figure 1: Example of a dimension partition tree T over $D = \{1, 2, 3, 4\}$

For example, in Figure 1, the tree T contains the nodes $\{\{1\}, \{2\}, \{3\}, \{4\}, \{1, 2\}, \{3, 4\}, \{1, 2, 3, 4\}\}$ and the corresponding tensors are $\{v_1, v_2, v_3, v_4, v_{1,2}, v_{3,4}, v_{1,2,3,4}\}$. Then, the resulting approximation v takes the form

$$v = v_{1,2,3,4}(v_{1,2}(v_1(\phi_1(x_1)), v_2(\phi_2(x_2)), v_{3,4}(v_3(\phi_3(x_3)), v_4(\phi_4(x_4)))))$$

where the $\phi_\alpha : \mathcal{X}_\alpha \to \mathbb{R}^{n_\alpha}, \alpha \in \{1, 2, 3, 4\}$, are some feature maps.
The tensors v_α are estimated by higher-order PCA for multivariate functions. In practice, PCA is realized on sample-based projections of the function u. To provide a final approximation with a prescribed error ε, i.e $\|u-v\|_{L^2_\mu(\mathcal{X})} \leq \varepsilon$, we use the so-called boosted optimal weighted least-squares

projection from [3]. With this choice, the stability of the sample-based projection is ensured almost surely with a number of evaluations of the function close to the interpolation regime.

In order to obtain an approximation error ε with the smallest number of samples N, adaptive strategies are proposed for the choice of the dimension tree T, the estimation of the empirical principal components and the selection of feature maps. More precisely, concerning the choice of the tree T, we present stochastic algorithms for tree optimization. The number of function's evaluations necessary for this tree optimization is small compared to a deterministic approach, as in [1]. We also propose a strategy which constructs adaptively the boosted weighted least squares projection using a sequence of nested spaces with increasing dimension, inspired from [4].
The performance of the proposed methods will be demonstrated on numerical test cases.

References

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Short biography – I graduated from Centrale Nantes with a specialization in applied mathematics and from the Technical University of Munich with a specialization in computational mechanics in 2017. I began a PhD thesis whose subject is "Low-rank approximation methods for complex uncertainty quantification problems". This thesis is a joint work between Centrale Nantes and the CEA DAM.