Statistical learning in tree-based tensor format

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Abstract:

Tensor methods are widely used tools for the approximation of high dimensional functions. Such problems are encountered in uncertainty quantification and statistical learning, where the high dimensionality imposes to use specific techniques, such as rank-structured approximations [1].

In this work, we introduce a statistical learning algorithm for the approximation in tree-based tensor format, which are tensor networks whose graphs are dimension partition trees (figure 1), of a function $f(X)$ which is typically expensive to evaluate. In uncertainty quantification, $X = (X_1, \ldots, X_d)$ is a set of d random variables modeling the uncertainties in a model (computational or experimental). Tree-based tensor formats include the Tucker format, the Tensor-Train format, as well as the more general Hierarchical tensor formats [4]. It can be interpreted as a deep neural network with a particular architecture [2].

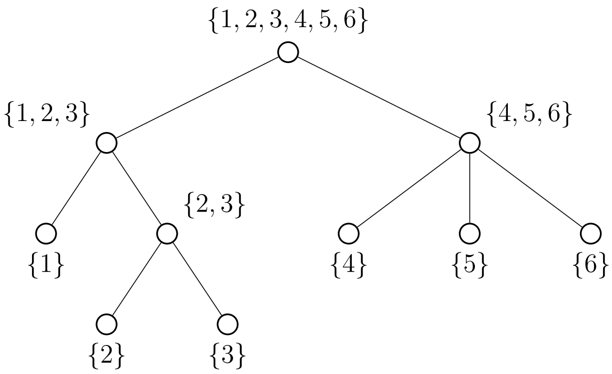

Figure 1: Example of a dimension partition tree T over $D = \{1, \ldots, 6\}$.

The proposed algorithm uses a training sample $\left\{(x^k, f(x^k)\right\}_{k=1}^N$ of N random evaluations of the function f to provide a tree-based tensor approximation $\hat{f}$, with adaptation of the tree-based rank by using a heuristic criterion based on the higher-order singular values to select the ranks to increase, and of the approximation spaces associated with the leaves of the tree.

The approximation is here obtained by least-squares regression on the training sample. Using the fact that tensors in tree-based format admit a multilinear parametrization, the parameters being denoted by $a_1, \ldots, a_M$, the minimization leads to the alternated solving, for each a_i, $i = 1, \ldots, M$, of

$$\min_{a_i} \frac{1}{N} \sum_{k=1}^{N} \left| f(x^k) - \Psi_i(x^k) a_i \right|^2 \quad (1)$$

until convergence. The $\Psi_i(x)$ are linear forms such that $\tilde{f}(x) = \Psi_i(x)a_i,\ i = 1, \ldots, M$. The adaptation of the approximation spaces previously mentioned is then performed by adding a ℓ_1 regularization term to (1), or by using a working-set strategy.

We then present a learning algorithm for the approximation under the form

$$f(x) \approx h(z_1, \ldots, z_m) \tag{2}$$

where h is a tensor in tree-based format and the $z_i = g_i(x)$, $1 \leq i \leq m$, are new variables. A strategy based on projection pursuit regression [3] is proposed to compute the mappings g_i and increase the effective dimension m. This algorithm can be useful to decrease the high dimension of a problem, by seeking adequate directions in the parameters space, or conversely to increase it, making tensor methods applicable for the approximation of univariate functions.

The methods are illustrated on different examples to show their efficiency and adaptability as well as the power of representation of the tree-based tensor format, possibly combined with changes of variables.

References

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Short biography – After a master's degree in computational mechanics at the Université de Nantes, I began a PhD thesis on the uncertainty quantification of the frequency response of vibrating underwater structures over a large frequency band, for which numerical simulations are expensive. This thesis is a part of the Joint Laboratory of Marine Technology between Centrale Nantes, Université de Nantes and the French company Naval Group, and of the Eval-π project.