Principal Component Analysis and boosted weighted least squares for training tree tensor networks

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One of the most challenging tasks in computational science is the approximation of high dimensional functions. Most of the time, only a few information on these functions is available, and approximating high-dimensional ones requires exploiting low-dimensional structures of these functions.
In this work, the approximation of a function u is built using point evaluations of the function, where the evaluations are selected adaptively. Such problems are encountered when the function represents the output of a black-box computer code, a system or a physical experiment for a given value of a set of input variables.
A multivariate function $u(x_1, ..., x_d)$ defined on a product set $\mathcal{X} = \mathcal{X}_1 \times ... \times \mathcal{X}_d$ can be identified with a tensor of order d. Here, we present an algorithm for the construction of an approximation of a function u in tree-based tensor format (tree tensor networks whose graphs are dimension partition trees). A low-order tensor is associated to each node of the dimension partition tree T, and this set of tensors totally parametrizes the approximation.
The algorithm relies on an extension of principal component analysis (PCA) to multivariate functions in order to estimate the tensors. In practice, PCA is carried on sample-based projections of the function u, using interpolation or least-squares regression.
To provide a stable projection, least-squares regression usually requires a high number of evaluations of u, which is not affordable in our context. This number of evaluations can be decreased thanks to a so-called boosted weighted least-squares method. This method combines an optimal weighted least-squares method proposed in [1] and a re-sampling technique. With a particular choice of weights and samples and through re-sampling, an approximation error of the order of the best approximation error is guaranteed using a moderate number of samples, of the order of the dimension of the approximation space.
Finally, we use this methodology in our algorithm to compare its efficiency with strategies using standard least-squares method or interpolation (as proposed in [2]).

Références

[1] Albert Cohen and Giovanni Migliorati, *Optimal weighted least-squares methods*, SMAI Journal of Computational Mathematics, 3:181203, 2017.

[2] Anthony Nouy, *Higher-order principal component analysis for the approximation of tensors in tree-based low-rank formats*, Numerische Mathematik, 2019.

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