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Mesh-free low-rank tensor representation of multivariate functions

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We introduce a mesh-free two-level hybrid Tucker tensor format for approximation of multivariate functions, which combines the product Chebyshev interpolation with the ALS-based Tucker decomposition of the tensor of Chebyshev coefficients. It allows to avoid the expenses of the rank-structured approximation of function-related tensors defined on large spatial grids, while benefiting from the Tucker decomposition of the rather small core tensor of Chebyshev coefficients. This leads to nearly optimal Tucker rank parameters which are close to the results for the well established Tucker-ALS algorithm applied to the large grid-based tensors. The rank parameters inherited from the Tucker-ALS decomposition of the coefficient tensor can be much less than the polynomial degrees of the initial Chebyshev interpolant obtained via a function independent basis set. Furthermore, the tensor product Chebyshev polynomials discretized on a tensor grid leads to a low-rank two-level orthogonal algebraic Tucker tensor that approximates the initial function with controllable accuracy. It is shown that our techniques could be gainfully applied to the long-range part of the electrostatic potential of multi-particle systems approximated in the range-separated tensor format. Error and complexity estimates of the proposed methods are presented. We demonstrate the efficiency of the suggested method numerically on examples of the long-range components of multi-particle interaction potentials generated by 3D Newton kernel for large bio-molecule systems and lattice-type compounds.

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