Towards efficient utilization of the canonical polyadic decomposition to approximate tensor networks in high accuracy electronic structure methods

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Abstract: It is well understood that accurate computer modeling of chemical properties and reactions via wavefunction-based methods is severely limited by the representation of physical quantities as dense, multi-index arrays (also known as higher-order tensors [HOTs]). In order to combat the storage and operational costs of using dense HOTs, costs which grow proportionally to the number of tensor indices, several forms of tensor decompositions have emerged as routes towards efficient sparse tensor representation and reduced scaling electronic structure theory methods[1,2]. In this work we utilize the canonical polyadic (CP) decomposition: a rank-sparse representation, akin to the singular value decomposition, that represents a tensor as a sum of component rank-one tensors. Application of the CP decomposition allows us to develop reduced scaling approximations of the most rate-limiting tensor networks in the Laplace-transform approximated perturbative triple correction to coupled cluster with single and double excitations [LT CCSD(T)] method. In this work we leverage standard and novel schemes to quickly and accurately generate CP approximations of Hamiltonian tensor quantities in high-cost tensor networks[3,4]. We demonstrate the effectiveness of these CP strategies by showing realized cost reduction of CP-based algorithms over canonical approaches for reasonable chemical systems while introducing a negligibly small degree of error into the computation of chemically relevant quantities.

References:

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