CHEBYSHEV APPROXIMATION OF FUNCTIONS AND FUNCTION COMPOSITION IN QUANTUM-INSPIRED NUMERICAL ANALYSIS

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This work deals with the problem of representing functions in matrix product states (MPS), also known as quantized tensor trains (QTT). These representations can circumvent the exponential scaling with respect to dimension suffered by the tensor representations of some categories of functions, known as the curse of dimensionality. Furthermore, it enables their subsequent use in quantum-inspired numerical methods^[1,2], which can yield up-to exponential advantages with respect to other conventional techniques. To this end, this work proposes an algorithm based on the Chebyshev approximation framework, relying on a finite precision non-linear algebra that enables linear combinations and multiplications of MPS. This algorithm avoids the exponential scaling of the standard approach based on the Schmidt decomposition, instead requiring polynomial resources. Moreover, it converges stably and according to the theoretical convergence properties of Chebyshev expansions, which are excellent for analytical and highly-differentiable functions. In its general form, this algorithm enables the compositions of generic univariate functions on arbitrary matrix product states. This enables it to encode multivariate functions whose algebraic structure is given by the composition of univariate ones. In addition, it can be generalized to compose multivariate functions, as well as to operate on matrix product operators (MPO).

This work evaluates the performance of the MPS/QTT Chebyshev approximation for a collection of univariate and multivariate functions. The results for the univariate functions show how the algorithm converges according to the theoretical convergence rates and requires computational resources that scale algebraically, both in time and memory. This provides exponential savings in memory with respect to their vector representation, and in time with respect to the standard approach based on the Schmidt decomposition. More precisely, the algorithm yields a sublinear runtime scaling with respect to the number of qubits of the MPS, and close-to-linear with the order of the approximating polynomial. This justifies its application for function composition, as well as its generalization to the multivariate case. In the multivariate scenario, the algorithm exhibits an analogous performance, showing stable convergence and requiring polynomial resources both in time and memory for functions with up-to 10 dimensions.



We compare the performance of this method with two other algorithms of the state-of-the-art, namely, multiscale interpolative constructions^[3] and tensor cross-interpolation (TCI)^[4]. Our findings show that, in the univariate case, the algorithm is less performant when loading univariate functions by one order of magnitude with respect to the former, and two with respect to the latter. However, as opposed to the former, it can be applied for other tasks, such as for generic function composition or for encoding multivariate functions in any qubit order; and as opposed to the latter, it requires two orders of magnitude less function evaluations, and shows advantageous scaling rates. Moreover, in the multivariate case, the algorithm shows a performance for loading multivariate analytical distributions that can be compared to that of TCI while using six orders of magnitude less evaluations.

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