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Generalization of the tensor renormalization group approach to 3-D or higher dimensions

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ABSTRACT

In this paper, a way of generalizing the tensor renormalization group (TRG) is proposed. Mathematically, the connection between patterns of tensor renormalization group and the concept of truncation sequence in polytope geometry is discovered. A theoretical contraction framework is therefore proposed. Furthermore, the canonical polyadic decomposition is introduced to tensor network theory. A numerical verification of this method on the 3-D Ising model is carried out.

1. Introduction

Tensor network model has become a promising method in simulating classical and quantum many body systems. This method represents physical quantities, such as, wave-function, or the exponential of a Hamiltonian, in terms of a multi-indexed tensor. Then we can calculate, physical observables, or partition functions, from a network of tensors. After contracting over this network, we can get physical behavior of our many body system. Examples of this approach is the matrix product state (MPS) [1,2] and projected entangled paired states (PEPS) [3].

The density matrix renormalization group (DMRG) [4] is a powerful method for 1-D quantum systems. For systems in dimensions larger than 1, the DMRG algorithm is known to scale exponentially with the system size. The tensor network correspondence of the DMRG, which is MPS, can be generalized to higher dimensions. Other generalizations such as multi-scale entanglement variational ansatz (MERA) [5] are also key aspects of the tensor network theory.

Compared with quantum Monte Carlo, which suffers from the sign problem, tensor network provides us a new way of doing calculations. Direct contraction of a tensor network, however, is not always possible. As a result, finding an organized way to approximate and contract a tensor network is an important aspect of the tensor network method. For example, we can group together some tensors systematically and contract some of our tensors and get a new coarse-grained tensor. The new tensor network shares the same symmetry with the original tensor network. This idea was explored by Levin and Nave [6]. They proposed this method for 2-D classical lattice models and use singular value decomposition (SVD) to do approximations. Their method has a similar spirit with the block spin method [7], and they call this method tensor renormalization group(TRG). It can be generalized to the so-called second renormalization group (SRG) [8], tensor network renormalization (TNR) [9], higher-order singular value decomposition (HOSVD) [10]. The way of contracting over the tensor network can also be applied to quantum models using the mapping between a d-dimensional quantum system and $d+1$ dimensional classical system [11]. Novel decompositions such as rank-1 decompositions was also proposed to tensor network theory [12].

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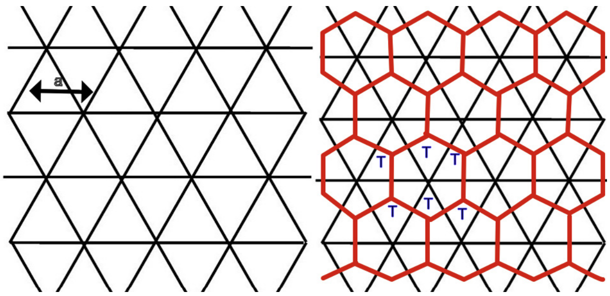

Fig. 1. The triangular Ising lattice and its tensor network (red). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

TRG proposed by Levin and Nave is for 2-D classical systems. For higher dimensional system, especially 3-D, calculations had been done, for example, as a variant of DMRG [13], as a new contraction strategy [14], and HOSVD [10]. Among these methods, HOSVD shares some similarities with TRG. Mathematically, HOSVD uses Tucker decomposition, which is a specific higher dimensional generalization of SVD. But we should notice that when their method is applied to 2-D system, the geometric structure of the contraction is different from TRG. Therefore it is necessary for us to consider the generalization TRG to higher dimensions.

In this paper, we propose a framework to do contraction systematically on tensor networks in higher dimensions. We also generalized TRG to higher dimensional tensor network. To achieve this goal, we introduce the canonical polyadic decomposition (CPD) into the tensor network method. The concept of tensor rank can also be defined using CPD, therefore, CPD is also called tensor rank decomposition. Our method reduces to 2D-TRG when it is applied to 2-D tensor network, which is a result of the fact that SVD is the 2-D version of CPD.

We apply our method to a 3-D cubic tensor network. The concept of the dual tensor network is also proposed. To make the contraction process iterate, the tensor network has to go from the original tensor network to its dual tensor network, then dual back. The dual of the dual tensor network has the same geometric structure with the original tensor network.

Mathematically, we propose a correspondence between TRG and the concept of truncation sequence in polytope geometry. The tensor network transforms in the same way as the truncation of a polyhedron(polytope in 4-D or higher). And the tensor CPD geometrically correspond to the truncation of the corner of a polyhedron. TRG in 2-D can also be understood in the framework of dual tensor network and truncation sequence.

This paper is organized as follows. Section 2 reviews the tensor renormalization group method in 2-D. Section 3 generalizes the concept of TRG to 3-D, CPD is introduced and details about the renormalization process are discussed. Section 4 shows some simulation results about this 3-D tensor renormalization group method. Section 5 proposes the similar method in higher dimensions. Section 6 discusses some applications and problems with this method.

Regarding the terminology, we need to mention some points that may be ambiguous. The word 'truncation' means either the numerical truncation of the singular values of a tensor(matrix) or the geometric truncation of a polytope. The word 'honeycomb' means either the 2-D honeycomb lattice or tessellation of a higher dimensional space.

2. Tensor renormalization approach for 2-D

2.1. Classical Ising model and tensor network

Let us first review 2-D TRG and discuss its geometric meanings. For a classical lattice system, one can find its tensor network representation. For example, both triangular and kagome lattice can be mapped to a honeycomb tensor network. A honeycomb tensor network may correspond to two Ising model: (1) a triangular lattice Ising model, see Fig. 1. (2) a kagome lattice one, see Fig. 2.

By connecting the centers of the triangles for both lattices, we get a honeycomb tensor network. In these Ising models, the spins live on the vertices and interactions lives on the lines, while for the tensor network, each tensor corresponds to a triangle and is represented by T_{ijk}. The three indices of the tensor T_{ijk} correspond to three spins of the Ising model.

The partition function of a system can be represented by

$$Z = \sum_{spins} e^{-\beta H(\sigma)} = \sum_{indices} T_{ijk}T_{jpq}T_{kab}T_{kmn}\ldots. \tag{1}$$

Here $\beta = (k_bT)^{-1}$, $H(\sigma)$ is the Hamiltonian of the Ising model, and k_b is the Boltzmann constant.

$$H(\sigma) = -\sum_{\langle ij\rangle} J\sigma_i\sigma_j - \mu h \sum_i \sigma_i. \tag{2}$$