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Nearest-neighbor interaction systems in the tensor-train format

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ABSTRACT

Low-rank tensor approximation approaches have become an important tool in the scientific computing community. The aim is to enable the simulation and analysis of high-dimensional problems which cannot be solved using conventional methods anymore due to the so-called curse of dimensionality. This requires techniques to handle linear operators defined on extremely large state spaces and to solve the resulting systems of linear equations or eigenvalue problems. In this paper, we present a systematic tensor-train decomposition for nearest-neighbor interaction systems which is applicable to a host of different problems. With the aid of this decomposition, it is possible to reduce the memory consumption as well as the computational costs significantly. Furthermore, it can be shown that in some cases the rank of the tensor decomposition does not depend on the network size. The format is thus feasible even for high-dimensional systems. We will illustrate the results with several guiding examples such as the Ising model, a system of coupled oscillators, and a CO oxidation model.

1. Introduction

Over the last years, the interest in low-rank tensor decompositions has been growing rapidly and several different tensor formats such as the canonical format, the Tucker format, and the TT format have been proposed. It was shown that tensor-based methods can be successfully applied to many different application areas, e.g. quantum physics [1,2], chemical reaction dynamics [3–7], stochastic queuing problems [8,9], machine learning [10–12], and high-dimensional data analysis [13]. The applications typically require solving systems of linear equations, eigenvalue problems, ordinary differential equations, partial differential equations, or completion problems. One of the most promising tensor formats for these problems is the so-called *tensor-train format* (TT format) [14–16], a special case of the *hierarchical Tucker Format* [17–20]. In this paper, we will consider in particular high-dimensional interaction networks described by a *Markovian master equation* (MME). The goal is to derive systematic TT decompositions of high-dimensional tensors for interaction networks that are only based on nearest-neighbor interactions. In this way, we want to simplify the construction of tensor-train representations, which is one of the most challenging tasks in the tensor-based simulation of interaction networks. The resulting TT decomposition can be easily scaled to describe different state space sizes, e.g. number of reaction sites or number of species. The complexity of a tensor train is determined by the TT ranks. Not only the memory consumption of the tensor operators is affected by the ranks, but also the costs of standard operations such as the calculation of norms and the runtimes of tensor-based solvers.

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Many applications require solving high-dimensional systems of linear equations of the form $\mathbf{A}\cdot\mathbf{T}=\mathbf{U}$, where $\mathbf{A}$ is a linear TT operator and $\mathbf{T}$ and $\mathbf{U}$ are tensors in the TT format. The efficiency of algorithms proposed so far for solving such systems such as ALS, MALS, or AMEn [21,22,5] depends strongly on the TT ranks of the operator. As a result, it is vitally important to be able to generate low-rank representations of $\mathbf{A}$. This can be achieved by truncating the operator, neglecting singular values that are smaller than a given threshold ε, or by exploiting inherent properties of the problem. Our goal is to derive a low-rank decomposition which represents the operator $\mathbf{A}$ associated with nearest-neighbor interaction networks exactly, without requiring truncation.

Finding a TT decomposition of a given tensor is in general cumbersome, in particular if the number of cells is not determined a priori. In [7], we derived a systematic decomposition for a specific reaction system and it turned out that the underlying idea can be generalized to describe a larger class of interaction systems. The only assumption we make is that the system comprises only nearest-neighbor interactions. The number and types of the cells as well as the interactions between these cells may differ. Moreover, systems with a cyclic network structure can be represented using the proposed TT decomposition. One of the main advantages of the presented decomposition is that the TT ranks of homogeneous systems do not depend on the number of cells of the network.

The paper is organized as follows: In Section 2, we give a brief overview of the TT format and define a special core notation. Furthermore, nearest-neighbor interaction systems defined on a set of cells and Markovian master equations are introduced. In Section 3, a specific TT decomposition is derived exploiting properties of nearest-neighbor interaction systems. In Section 4, we use this TT decomposition for Markovian master equations in the TT format and present numerical results. Section 5 concludes with a brief summary and a future outlook.

2. Theoretical background

In this section, we will introduce the concept of tensors and different tensor decompositions, namely the canonical format and the TT format. Furthermore, we will define interaction systems that are based only on nearest-neighbor couplings. We will distinguish between homogeneous and heterogeneous systems as well as between cyclic and non-cyclic systems.

2.1. Tensor formats

Tensors, in our sense, are simply multidimensional generalizations of vectors and matrices. A tensor in full format is given by a multidimensional array of the form $\mathbf{T}\in\mathbb{R}^{n_1\times\cdots\times n_d}$ and a linear operator by $\mathbf{A}\in\mathbb{R}^{(n_1\times n_1)\otimes\cdots\otimes(n_d\times n_d)}$. The entries of a tensor are indexed by $\mathbf{T}_{x_1,\ldots,x_d}$ and the entries of operators by $\mathbf{A}_{x_1,y_1\ldots,x_d,y_d}$. In order to mitigate the curse of dimensionality, that is, the exponential growth of the memory consumption in d, various tensor formats have been proposed over the last years. Here, we will focus on the TT format. The common basis of various tensor formats is the tensor product which enables the decomposition of high-dimensional tensors into several smaller tensors.

Definition 2.1. The *tensor product* of two tensors $\mathbf{T}\in\mathbb{R}^{m_1\times\cdots\times m_d}$ and $\mathbf{U}\in\mathbb{R}^{n_1\times\cdots\times n_e}$ defines a tensor $\mathbf{T}\otimes\mathbf{U}\in\mathbb{R}^{(m_1\times\cdots\times m_d)\times(n_1\times\cdots\times n_d)}$ with

$$(\mathbf{T}\otimes\mathbf{U})_{x_1,\ldots,x_d,y_1,\ldots,y_e}=\mathbf{T}_{x_1,\ldots,x_d}\cdot\mathbf{U}_{y_1,\ldots,y_e},$$

where $1\leq x_k\leq m_k$ for $k=1,\ldots,d$ and $1\leq y_k\leq n_k$ for $k=1,\ldots,e$.

The tensor product is a bilinear map. That is, if we fix one of the tensors we obtain a linear map on the space where the other tensor lives (see Appendix A). The initial concept of tensor decompositions was introduced in 1927 by Hitchcock [23], who presented the idea of expressing a tensor as the sum of a finite number of *rank-one tensors* (or *elementary tensors*).

Definition 2.2. A tensor $\mathbf{T}\in\mathbb{R}^{n_1\times\cdots\times n_d}$ is said to be in the *canonical format* if

$$\mathbf{T}=\sum_{k=1}^{r}\left(\mathbf{T}^{(1)}\right)_{k,:}\otimes\cdots\otimes\left(\mathbf{T}^{(d)}\right)_{k,:}, \tag{1}$$

with *cores* $\mathbf{T}^{(i)}\in\mathbb{R}^{r\times n_i}$ for $i=1,\ldots,d$. The parameter r is called the *rank* of the decomposition.

Remark 2.3. Given a canonical tensor $\mathbf{T}$ as defined in (1), a cyclic permutation of the cores yields a tensor whose indices are permuted correspondingly. That is, if we define

$$\tilde{\mathbf{T}}=\sum_{k=1}^{r}\left(\mathbf{T}^{(m)}\right)_{k,:}\otimes\cdots\otimes\left(\mathbf{T}^{(d)}\right)_{k,:}\otimes\left(\mathbf{T}^{(1)}\right)_{k,:}\otimes\cdots\otimes\left(\mathbf{T}^{(m-1)}\right)_{k,:},$$

with $1\leq m\leq d$, we obtain

$$\tilde{\mathbf{T}}_{x_m,\ldots,x_d,x_1,\ldots,x_{m-1}}=\mathbf{T}_{x_1,\ldots,x_{m-1},x_m,\ldots,x_d}.$$