

令和 4 年 6 月 13 日現在

機関番号：82401

研究種目：若手研究

研究期間：2020～2021

課題番号：20K19875

研究課題名（和文）Structured Tensor Approximation under Kronecker Graph and Its Application on Hydrological Data

研究課題名（英文）Structured Tensor Approximation under Kronecker Graph and Its Application on Hydrological Data

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交付決定額（研究期間全体）：（直接経費） 3,200,000円

研究成果の概要（和文）：高次元の課題解決において、テンソルモデルは様々な分野での活用が進んでいる。しかし、テンソルネットワーク構造探索（TN-SS）やテンソル学習ダイナミクス（TLD）の解析など未解明の問題が多く残されている。TN-SSにおいては、本研究でサンプリングに基づくアルゴリズムによって、最適なテンソルネットワーク構造を獲得することが確認された。さらに、探索空間の理論解析を加えることで、2つの効率的なサンプリングスキームを提案した。時系列予測に向けたTLDの分析では、モデルの記憶機構とテンソル次数の関係を明らかにした。加えて、テンソルによるロングメモリ効果を最大化できる新たな予測手法を提案した。

研究成果の学術的意義や社会的意義

Tensor is a promising framework, which tightly bonds many scientific fields for the human society. The results of the project reveal how the tensor structures impact its behavior in machine learning and practically provides methods to maximize the performance in real-world applications.

研究成果の概要（英文）：Tensor models have been widely applied to resolving extremely high-dimensional tasks in various fields. However, there remain many unexplored problems for tensors, particularly for tensor network structure search (TN-SS) and the analysis of the tensor learning dynamics (TLD). In this project, we conduct a thorough investigation of the preceding issues. For TN-SS, we found that the optimal tensor network structure can be obtained by sampling-based algorithms, for which we propose two efficient sampling schemes with theoretical analysis of the search space. For analyzing TLD in time series forecasting, our study reveals the relationship between the models' memory mechanism and the tensor orders. We also propose a new forecasting method called the fractional tensor recurrent unit (fTRU), which can maximize the benefit of the long-memory effect by tensors. Extensive experimental results on real-world data demonstrate the usefulness of the methods studied in the project.

研究分野：machine learning

キーワード：tensor network

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1 . 研究開始当初の背景

Over the years, tensor decomposition has been widely concerned in various scientific and technical fields. It enables us to resolve extremely high-dimensional problems with acceptable computational and storage costs. Tensor network (TN) originated in quantum physics as a workhorse for calculating many-body systems and has also been widely applied to machine learning tasks in recent years. Compared with the conventional tensor decomposition models such as CP, Tucker, or block-term decomposition (BTD), TN provides more flexible structures associated with arbitrary simple graphs. As an expected consequence, many studies have theoretically and numerically proved the advanced expressive power of TNs in extensive machine learning tasks.

However, there remain unexplored problems up until now for TNs due to the inherent irregularity of the TN structures and the non-linear (multi-linear, in fact) behaviors in learning tasks. For model selection, practitioners are faced with a notorious challenge when applying TNs to practical tasks: how to efficiently select the optimal TN structures from a massive quantity of candidates? Resolving the problem is theoretically NP-hard, and the solution space is unacceptably huge even for a small-scale problem, so trivial algorithms such as the exhaustive search become unavailable for selecting the optimal TN structure in practice. The TN-based models cannot achieve the ideally expected learning performance due to the improper selection of TN structures.

The analysis of the learning properties of tensor models is also lacking so far, particularly for time series forecasting. The reason is mainly twofold: theoretically, the non-linear recurrence makes the understanding of the tensor models more challenging than the existing linear recurrent models; numerically, an “over-large” tensor order would lead to the model being unstable in both the training and inference phase. Consequently, the TN-based models for time series forecasting fail to be the mainstream in sequence tasks, even though there has been much literature that empirically proves the tensor models' effectiveness in practice. Taken together, these facts thus motivate the study of this project, for the more efficient utilization of tensor (networks) in machine learning and a deeper understanding of their learning properties.

2 . 研究の目的

This project aims to conduct a thorough investigation of the preceding problems from both the theoretical and empirical aspects. We summarize the main research targets of this project as follows:

- (1) We aim to propose practically efficient algorithms for resolving the problem of *tensor network structure search* (TN-SS), with a theoretical analysis of the properties of the irregular structure spaces;
- (2) For the time series forecasting task, we are to theoretically analyze *the learning behaviors for the tensor-based recurrent models*, discussing the potential advantage compared with the classic models. Furthermore, we are going to develop more efficient methods, improving the prediction accuracy in the sequence tasks;
- (3) We explore *novel machine learning applications*, in which the low-rank tensor (network) models have the potential to improve the performance of learning tasks.

3 . 研究の方法

In the project, we conduct a thorough investigation of the research targets from both the theoretical and empirical aspects. For tensor network structure search (TN-SS), the theoretical studies on the properties of the structures, such as the counting and geometry of the search space, were derived using the elementary instruments from group and graph theory. The good modeling for symmetries by group theory reveals the essence of TN structures and helps develop practical searching algorithms. On the empirical side, various combinatorial optimization methods were explored and refined, aided by the established theory in the project for more efficient searching routines.

In the tensorial forecasting of time series, the learning dynamics of the tensor models were studied using tools from stochastic differential equations and stochastic processes. We focused on analyzing the correlation properties of the processes generated by the tensor recurrent models, which implies the long-term memory mechanism of the model and is crucially important for the forecasting task. Empirically, we study the practically stable tensor-recurrent models using neural sub-networks to control key model parameters like the tensor order that determines the system's stability. The computation required in the experiments was carried out at the Riken AI Deep learning Environment (RAIDEN).

4. 研究成果

(1) **The optimal TN structures can be obtained via well-designed random-sampling methods.** For the problem of tensor network structure search (TN-SS), we focused on searching for unexplored TN topology and “mode-vertex” mappings for tensor learning tasks. In the work, we first claim that the issue can be practically tackled by evolutionary algorithms (EAs) in an affordable manner. We encode the complex topological structures into binary strings and develop a simple genetic meta-algorithm to search for the optimal topology in Hamming space. Based on this result, we further propose a more efficient local-sampling algorithm, in which the searching is done by randomly sampling in a neighborhood established in our theory, and then recurrently updating the neighborhood until convergence. On the theoretical side, we prove the counting and metric properties of spaces for searching the optimal “mode-vertex” mappings, revealing for the first time the impact of the symmetry of TN topology on these unique properties. The experimental results demonstrate that the proposed methods can effectively discover the optimal TN topology and other structures in real-world decomposition/completion/learning tasks. More research details can be found in papers presented at the international conference on machine learning (ICML) in the years 2020 and 2022, respectively.

(2) **Tensor order plays a crucial role in the memory mechanism of tensor recurrent models.** Targeting the time series forecasting task, we first conduct a thorough investigation of the memory mechanism of the tensor recurrent model. Theoretically, we prove that a large tensor order is an essential condition to achieve the long memory effect, yet it could lead to unstable dynamical behaviors. Empirically, we tackle this issue by extending the tensor order from discrete to a differentiable domain, proposing a new model called fractional tensor recurrent unit (fTRU), such that it is efficiently learnable from a variety of datasets. We experimentally show (see Figure 1) that using the proposed model we achieve competitive performance compared to various advanced RNNs in several forecasting tasks, with adaptive memory to ensure stability. This part of the work is presented at the international conference on artificial intelligence and statistics (AISTATS) 2021.

Meanwhile, we also studied the potential capability of tensor models for time series forecasting in the application of multi-modal sentiment analysis (MSA), which has been widely investigated in both computer vision and natural language processing. We found that the studies on the imperfect data, especially with missing values, were still far from successful and challenging, even though such an issue is ubiquitous in the real world. To this end, we propose a novel network architecture termed Time Product Fusion Network (TPFN), which takes the high-order statistics over both modalities and temporal dynamics into account. We construct the fused features by the outer product along with adjacent time steps, such that richer modal and temporal interactions are utilized. In addition, we claim that the low-rank structures can be obtained by regularizing the Frobenius norm of latent factors instead of the fused features. Experiments on CMU-MOSI and CMU-MOSEI datasets show that TPFN can compete with state-of-the-art approaches in multimodal sentiment analysis in cases of both random and structured missing values. This part of the work is presented at the European conference on computer vision (ECCV) 2020.

(3) Low-rank TN methods achieve state-of-the-art performance for image completion and steganography problems. In the image completion problem, we propose a new approach to exploit the low TR-rank structure in the work. Specifically, we first introduce a balanced unfolding operation called tensor circular unfolding, by which the relationship between TR rank and the ranks of the tensor unfoldings is theoretically established. Using this new unfolding operation, we propose an algorithm to exploit the low TR-rank structure by performing parallel low-rank matrix factorizations to all circularly unfolded matrices. The extensive experiments have demonstrated that the proposed algorithm can achieve outstanding performance using a much smaller TR rank than conventional TR-based completion algorithms; meanwhile, the computational cost is reduced substantially.

We also explore a new application for tensor decomposition, *i.e.*, information steganography, which is a family of techniques that hide secret messages into a carrier; thus, the messages can only be extracted by receivers with a correct key. In this work, we explore the room introduced by the low-rank property of natural signals (*i.e.*, images, audios), and propose a training-free model for efficient information steganography, which provides a capacity of hiding full-size images into carriers of the same spatial resolution. The key to the proposed method is to *randomly shuffle* the secrets and carry out a simple reduction summation with the carrier. In information recovery, the secret images can be reconstructed by solving a convex optimization problem similar to the ordinary tensor decomposition. In the experimental analysis, we carry out two tasks: concealing a full-RGB-color image into a gray-scale image; concealing images into music signals. The results confirm the ability of our model to handle massive secret payloads.

5. 主な発表論文等

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〔図書〕 計0件

〔産業財産権〕

〔その他〕

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6. 研究組織

氏名 (ローマ字氏名) (研究者番号)	所属研究機関・部局・職 (機関番号)	備考
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7. 科研費を使用して開催した国際研究集会

〔国際研究集会〕 計0件

8. 本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関
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