HOTTBOX: Higher Order Tensor ToolBOX for the Analysis of Multi-way Data

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Abstract

HOTTBOX is a Python library for exploratory analysis and visualisation of multi-dimensional arrays of data, also known as tensors. The library includes methods ranging from standard multi-way operations and data manipulation through to multi-linear algebra based tensor decompositions. HOTTBOX also comprises sophisticated algorithms for generalised multi-linear classification and data fusion, such as Support Tensor Machine (STM) and Tensor Ensemble Learning (TEL). For user convenience, HOTTBOX offers a unifying API which establishes a self-sufficient ecosystem for various forms of efficient representation of multi-way data and the corresponding decomposition and association algorithms. Particular emphasis is placed on scalability and interactive visualisation, to support multidisciplinary data analysis communities working on big data and tensors. HOTTBOX also provides means for integration with other popular data science libraries for visualisation and data manipulation. The source code, examples and documentation can be found at https://github.com/hottbox/hottbox.

1 Introduction

Tensors are higher order generalisations of matrices and vectors, which represent data in the form of a multi-way array. This is achieved through indexing by an arbitrary number of indices (tensor order), whereby different physically meaningful properties and characteristics are ideally attributed to different dimensions (modes) of an N-dimensional array. Such data representation offers a whole host of opportunities for discovering latent dependencies and intrinsic structures in data. Owing to the inherent flexibility and horizontal scalability of multi-way analysis, tensors have found application in a diverse range of disciplines, from very theoretical ones, such as physics and numerical analysis [1, 2], to the more applied areas, such as face recognition [3], separation of unknown sources of brain activity [4], cross-language information retrieval [5] and computational neuroscience [6, 7], to mention but a few. However, both the analysis and wider adoption of tensors are still being hampered by a lack of software tools which offer interactive scientific visualisation throughout the analysis.

Over the past decade, extensive literature has been published on multi-way analysis, owing to the ability of tensor decompositions to alleviate the “Curse of Dimensionality”, such techniques range from fundamental principles behind tensor decompositions [8, 9] to
quite advanced and sophisticated techniques such as tensor networks [10]. In addition, we have witnessed a rapid growth of the amount of data being generated and collected, together with the corresponding storage capabilities and processing power, these are readily available through either local or cloud computing to users even outside of academia and industry. The multi-way analysis community has responded with the development of open source packages [11, 12, 13, 14] in order to mitigate, for a generally knowledgeable user, most of the technicalities behind implementation of tensor decompositions, alongside the corresponding statistical methods and data analysis techniques. Existing publicly available libraries are mainly designed as general purpose toolboxes comprising fundamental tensor decompositions, e.g. Canonical Polyadic Decomposition (CPD), Tucker Decomposition (TKD) and Tensor Train Decomposition (TT), with a focus on efficient performance of such methods.

The Higher Order Tensor ToolBOX (HOTTBOX), presented here, is an open source toolbox for tensor decompositions, statistical analysis, visualisation, feature extraction, regression and non-linear classification of multi-dimensional data. The package is written in Python and was conceived with the aim to serve as a self-contained library which allows for seamless integration with other popular data science packages for data wrangling, together with offering unique visualisation capability suitable for non-experts and multidisciplinary research communities. The HOTTBOX has already been rolled out as a research tool and for educational purposes [15] and it is our hope that it will both help demystify tensor decompositions for various communities active in the area, and also attract the curious reader to gain experience with multi-way analysis.

2 Background: Available software for multi-linear operations

Over the past years, several libraries for dealing with multi-dimensional data have emerged, including:

- **Tensor Toolbox** [11], one of the first attempts to provide users with classes and functions for manipulating dense, sparse and structured tensors as well as fundamental tensor decompositions using MATLAB’s object-oriented features;

- **Tensorlab** [12], which offers various tools for tensor computations and complex optimisations. In addition, it also implements a number of algorithms dealing with large-scale datasets and more advanced factorisations, such as the LL1 and Block Term Decomposition (BTD) [16, 17], and supports quite intuitive tools for basic visualisations of N-dimensional data.

Both these toolboxes are well structured and provide extensive documentation supported with various examples; they also require a proprietary MATLAB platform. Existing packages written in Python include:

- **TensorLy** [13], which was developed with simplicity in mind and has a flexible backend system which allows to perform tensor decomposition algorithms at scale and over a range of hardware setups. TensorLy also comprises implementations of some machine learning approaches, but its main focus remains on optimised and efficient performance;

- The **TensorD** toolbox [14] was designed as a highly modular piece of software, specifically tailored to the most prominent machine learning framework, the TensorFlow.
Although it allows us to transform an idea into a result very quickly, it supports implementations of only CPD and TKD.

Several other libraries exist which primary focus on the Tensor Train Decomposition (TTD), a tensor factorisation originally introduced by a research group from the Skolkovo Institute of Science and Technology in 2011. The same group also released a Python implementation of their algorithms within a dedicated toolbox whose functionalities were then extended to support utilisation of hardware acceleration for efficient computations, batch processing and automatic differentiation [18]. Another package for tensor network learning with PyTorch takes a somewhat orthogonal approach to establishing a common interface, where the existing multi-linear models, i.e. CPD, TKD, TT, are represented as a particular case of tensor networks [10]. Thus, decomposing, manipulating, and reconstructing tensors can be (to some extent) abstracted away from the particular decomposition format.

To summarise, while all of the aforementioned libraries and projects have found their place within multi-way data analysis, the HOTTTBOX takes a step further by:

- Utilising tensors not only as N-dimensional arrays, but also exploiting complementary meta-information about the data a tensor represents;
- Offering scalable visualisation tools, at every stage of the analysis, to facilitate ease of analysis, multi-disciplinary efforts or educational purposes;
- Being focused on unifying the machine learning approaches which are specific to inherently multi-dimensional data.

3 Ecosystem of HOTTTBOX

Various types of data can be represented in the form of an N-dimensional array. Most often, this is achieved through a combination of mathematical construction and experimental design. For example, tensors can be constructed from:

- Time-frequency representation of each channel that records brain activity during a particular task or stimulus, that is, each slice on the left-most panel in Fig. 1[19][20];
- A video clip can be broken down into a set of consecutive frames which are stacked into a tensor, as in the middle panel in Fig. 1[21][22];
- Optical motion capture system that contains several markers, each of which can record information about position change in a 3-D space over a period of time, as illustrated in the right most-panel in Fig. 1[23][24].
3.1 Core structural components of HOTTBOX

Each dimension within an N-dimensional array can be associated with a certain property, or mode of the raw data. At the same time, this characteristic is described by a set of distinct features. To show this, assume that a simple data rearrangement procedure (e.g. folding, unfolding) of the raw data was performed which yielded a different view of data at hand. However, such manipulation does not change the original properties of the underlying data array, but instead it changes the relationships between models. We shall refer to such transformation of a “raw” N-dimensional data as a change of state. The HOTTBOX ecosystem therefore establishes the following principles and objects:

- **Mode** of the tensor is defined by the name of the property it represents and names of the features that describe this property;

- **State** of the tensor is defined by transformations applied to the data array;

- **Meta-data** about a tensor is a record of information about the modes and the state it is currently in.

Oftentimes, N-dimensional data contains a considerable amount of repetitive and redundant information. By applying different numerical methods, i.e. tensor decompositions, this information can be represented in a more compact and efficient way. There are three major conceptually different factorisation types and computational algorithms associated with tensors that are part of HOTTBOX:

- **Kruskal form** represents the original data as a list of matrices, each of which corresponds to a particular dimension of an array. It also imposes a one-to-one relation between column vectors of these factor matrices;

- **Tucker form** is similar to Kruskal form, but every vector within one factor matrix is related to all vectors of the other factor matrices through a core tensor;

- **Tensor Train form** represents a tensor as a set of sparsely interconnected matrices and core tensors of low order, and therefore only adjacent components have explicit relation.
Figure 3: A conceptual diagram of the Tensor Ensemble Learning (TEL) framework within HOTTBOX. Each N-dimensional data sample (top left) from the original dataset is represented through either TensorCPD or TensorTKD (top right). The so-extracted components are reorganised and form a series of new datasets, each containing an incomplete information about the original sample (middle). An ensemble of machine learning algorithms is then employed, whereby each base learner generates an independent hypothesis which then used for “voting” in order to form a collective decision (bottom).

It is important to understand that the characteristics of modes of N-dimensional data remain the same regardless of the form used for their representation. Therefore, to suit the inherent characteristics of tensors, HOTTBOX provides a unified API which is very convenient as it:

- Allows for switching between different tensor forms seamlessly;
- Preserves information about the underlying tensor characteristics;
- Gives an opportunity to utilise meta-information with ease.

The core structural components of HOTTBOX are therefore the Tensor, TensorCPD, TensorTKD and TensorTT classes which bring together the raw, Kruskal, Tucker, and Tensor Train formats, respectively.

3.2 Supported algorithms

One aspect of the HOTTBOX library is to facilitate the usage of a wide range of existing numerical methods which are available for analysis of inherently multi-dimensional data. The HOTTBOX splits implementation of such algorithms into several modules dedicated to different aspects of multi-way analysis, as follows:
Figure 4: An example of a dashboard for visualising the TensorTKD. It fully exploits the relationships between components and utilises the associated meta-information.

- The tensor factorisation module comprises of implementations of fundamental tensor decompositions which include the Canonical Polyadic, Higher Order Singular Value and Tensor Train decompositions \[8\] \[25\] \[26\] that can be used to represent a “raw” multi-modal data as one of the structures covered in Section 3.1. A set of these algorithms is further extended with different variations which have been proposed in the literature on optimised processing of multi-dimensional arrays. For example, the Higher Order Orthogonal Iteration (HOOI) Decomposition \[27\] aids the actual computation of the best multi-linear approximation, while the Randomised Canonical Polyadic Decomposition \[28\] significantly reduces both memory requirements and computational speed, without sacrificing precision of the CP factorisation;

- Inside the data fusion and feature extraction module, the user can find the Coupled Matrix and Tensor factorisation \[29\] and PARAFAC2 \[30\] routines. Both can be employed to jointly analyse a multi-way array with a matrix or a collection of matrices that share a common mode (which describes similar data properties) in order to extract a latent structure that governs the underlying processes. Despite the latter model being able to simultaneously factorise a collection of only 2-dimensional structures, PARAFAC2 is still attributed to multi-way analysis as a variant of the CP representation with relaxed constrains;

- The classification and regression module includes implementations of the Least Squares Support Tensor Machine (LSSTM) and Tensor Ensemble Learning (TEL) algorithms (illustrated in Fig. 3) which respectively generalise concepts and ideas of the existing popular “flat-view” matrix frameworks, i.e. Support Vector Machine and Ensemble Learning frameworks \[10\] \[31\] to their tensor counterparts, such as Support Tensor Machine (STM). Thus, the LSSTM and TEL can be seen as a natural extension to the case of tensor-valued data samples.

The HOTTBOX is designed with the aim to offer easy integration of other emerging ML routines for Big Data.

### 3.3 Interactive visualisations

A key benefit of having a common API in our HOTTBOX library is that it provides us with the means to integrate the multi-linear structures with external popular libraries
that serve completely orthogonal purposes, e.g. data wrangling and visualisation. The latter is particularly important for exploratory data analysis, and when displaying various forms of tensor representations. This is completely different from commonly used toolboxes, as current approaches require a considerable amount of repetitive work to achieve an acceptable and effective visualisation result. To this end, in order to accommodate many versatile forms of efficient representations, the HOTTBOX provides users with an interactive dashboard. Fig. 4 illustrates such a visualisation with the user interface for a “raw” N-dimensional array factorised into the Tucker form. Due to the nature of this representation, different modes and components correspond to different properties that can be plotted using various types of graphs available in the dropdown menu. Although a set of options is predefined, it can be easily extended to suit a particular need of a user. In this way, a typically very large number of cross-modal relations intrinsic to the components of Tucker form (or other forms of efficient representations) can be explored with the use of sliders. Finally, meta-information is extracted and embedded as figure titles, to keep track of the design sequence.

Remark. Fig. 4 merely displays synthetic data for illustrational purposes, where each panel visualises a single column vector from three different factor matrices that would have been obtained through either CPD or TKD of brain activity represented in the form of a third order tensor.

3.4 Statistical toolbox

The HOTTBOX also provides classes and functions for the estimation of Tensor-Valued Gaussian statistical models. The inherent notion of tensor-valued probability density function makes this module suitable for a large variety of use-cases that aim to model interactions between real-world tensor data samples that are typically causal and probabilistic. Our implementation is compact, stemming from the Kronecker separability of the first- and second-order moments of the tensor-valued random variable, as elaborated in [32]. This property of tensor-valued statistical models provides an immediate reduction in the number of parameters required to represent a random process compared to the standard multivariate Gaussian model, as can be observed in Fig. 5.

The so-enabled exploitation of tensor-valued models is essential for alleviating the Curse of Dimensionality, that is, an exponential growth in data volume with an increase in the order of the tensor. At the same time, implementation of tensor-valued Gaussian statistical models within HOTTBOX equips researches and data analysts with the

Figure 5: The ratio of distinct parameters between the structured tensor model, $\eta_{\text{tensor}}$, and the classical unstructured model, $\eta_{\text{multi}}$, given by $\frac{\eta_{\text{tensor}}}{\eta_{\text{multi}}}$, for a varying mode dimensionality, $I$, and tensor order, $N$. 
essential tool for:

- Utilising Bayesian tensor inference methods;
- Straightforward consideration of a mixture of probabilistic models;
- Statistical and hypothesis testing through the tensor likelihood function;
- Employing class-conditional densities for classification tasks.

4 Conclusion and future work

The Higher Order Tensor ToolBOX (HOTTBOX) is a Python library dedicated to handling multi-dimensional data, which at its core employs a user-friendly approach to statistical analysis, visualisation, feature extraction, regression and non-linear classification paradigms. In this way, HOTTBOX can be used both by the data analytics communities and the multi-disciplinary communities which operate with inherently N-dimensional data arrays. The toolbox is equipped with a unit tests suite in order to meet the requirements on the integrity of the code base of the modern software. A particular emphasis has been placed on the importance of documentation\footnote{https://hottbox.github.io/develop} which is automatically updated to reflect the most recent development changes and to include the latest features. An interested reader can find more details in our publicly available repositories\footnote{https://github.com/hottbox/hottbox-tutorials} which contain a series of illustrative examples that can be tried out live in a cloud, for free and without any installation burden.

The ease of use makes the HOTTBOX also suitable for educational purposes, as a means to shed the light on the field of multi-linear analysis. For example, it has been used to facilitate the final year undergraduate and post graduate curriculum\footnote{https://github.com/IlyaKisil/dpm-coursework} within the courses “Adaptive Signal Processing and Machine Intelligence” and “Machine Learning for Finance”, at the authors’ home institution, enabling a seamless transition from the flat-view linear algebra to multi-linear analysis of tensors.
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