Learning Multiple Networks via Supervised Tensor Decomposition

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Abstract

We consider the problem of tensor decomposition with multiple side information available as interactive features. Such problems are common in neuroimaging, network modeling, and spatial-temporal analysis. We develop a new family of exponential tensor decomposition models and establish the theoretical accuracy guarantees. An efficient alternating optimization algorithm is further developed. Unlike earlier methods, our proposal handles a broad range of data types, including continuous, count, and binary observations, along with available features. We apply the method to diffusion tensor imaging data from human connectome project and identify the key brain connectivity patterns associated with available features. Our method will help the practitioners efficiently analyze tensor datasets in various areas. Toward this end, all data and code ~~has~~ have been made available to the public.

1 Introduction

Higher-order tensors have received increased attention across science and engineering. While most tensor decomposition methods are developed for a single tensor observation, scientific studies often collect side information, in the form of node features and interactions thereof, together with the tensor data. Such data problems are common in neuroimaging, network analysis, and spatial-temporal modeling. A popular example is in neuroimaging (Zhou et al., 2013). The brain connectivity networks are collected from a sample of individuals, accompanied by individual characteristics such as age, gender, and diseases status (see Figure 1a). Another example is in network analysis (Berthet and Baldin, 2020). Side information such as people's demographic information and friendship types are often available. In both examples, scientists are interested in identifing the variation in the data tensor (e.g., brain connectivities, social community patterns) that is affected by available features. These seemingly different scenarios pose a common yet challenging problem for tensor data modeling.

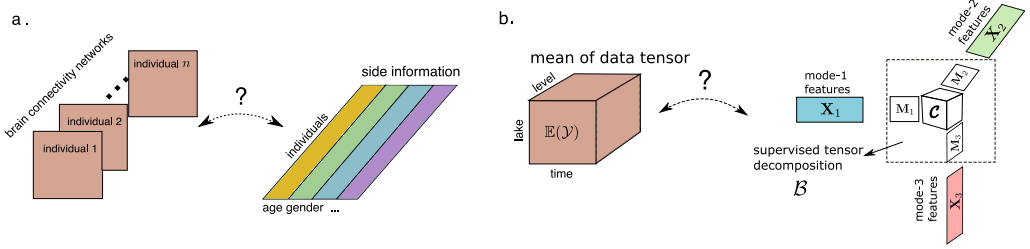

Figure 1: Examples of supervised tensor decomposition with interactive side information. (a) Network population model. (b) Spatio-temporal growth model.

In addition to the challenge of incorporating side information, many tensor datasets consist of non-Gaussian measurements. Classical tensor decomposition methods are based on minimizing the

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Frobenius norm of deviation, leading to suboptimal predictions for binary- or count-valued response variables. A number of supervised tensor methods have been proposed (Narita et al., 2012; Zhao et al., 2012; Yu and Liu, 2016; Lock and Li, 2018). These methods often assume Gaussian distribution for the tensor entries, or impose random designs for the feature matrices, both of which are less suitable for applications of our interest. The gap between theory and practice means a great opportunity to modeling paradigms and better capture the complexity in tensor data.

Our contribution. This paper presents a general model and associated method for decomposing a data tensor whose entries are from exponential family with interactive side information. We formulate the learning task as a low-rank tensor regression problem, with tensor observation serving as the response, and the multiple side information as interactive features. We blend the modeling power of generalized linear model (GLM) and the exploratory capability of tensor dimension reduction in order to take the best out of both worlds. Our methods greatly improves the classical tensor decomposition, and we quantify the gain in prediction through numerical experiments and data applications.

Notation. We follow the tensor notation as in Kolda and Bader (2009). The multilinear multiplication of a tensor $\mathcal{Y} \in \mathbb{R}^{d_1 \times \cdots \times d_K}$ by matrices $\boldsymbol{X}_k = [\![x^{(k)}_{i_k,j_k}]\!] \in \mathbb{R}^{p_k \times d_k}$ is defined as $\mathcal{Y} \times \{\boldsymbol{X}_1, \ldots, \boldsymbol{X}_K\} = [\![\sum_{i_1,\ldots,i_K} y_{i_1,\ldots,i_K} x^{(1)}_{j_1,i_1} \cdots x^{(K)}_{j_K,i_K}]\!]$, which results in an order-K $(p_1, \ldots, p_K)$-dimensional tensor. The inner product between two tensors of equal size is defined as $\langle \mathcal{Y}, \mathcal{Y}' \rangle = \sum_{i_1,\ldots,i_K} y_{i_1,\ldots,i_K} y'_{i_1,\ldots,i_K}$. For ease of notation, we allow basic arithmetic operators (e.g., $+, -$) and univariate functions $f\colon \mathbb{R} \to \mathbb{R}$ to be applied to tensors in an element-wise manner.

2 Proposed models and motivating examples

Let $\mathcal{Y} = [\![y_{i_1,\ldots,i_K}]\!] \in \mathbb{R}^{d_1 \times \cdots \times d_K}$ denote an order-K data tensor. Suppose the side information is available on each of the K modes. Let $\boldsymbol{X}_k = [\![x_{ij}]\!] \in \mathbb{R}^{d_k \times p_k}$ denote the feature matrix on the mode $k \in [K]$, where x_{ij} denotes the j-th feature value for the i-th tensor entity, for $(i, j) \in [d_k] \times [p_k]$, $p_k \leq d_k$. We assume that, conditional on the features $\boldsymbol{X}_k$, the entries of tensor $\mathcal{Y}$ are independent realizations from an exponential family distribution, and the conditional mean tensor admits the form

$$\mathbb{E}(\mathcal{Y} | \boldsymbol{X}_1, \ldots, \boldsymbol{X}_K) = f\left(\mathcal{C} \times \{\boldsymbol{X}_1 \boldsymbol{M}_1, \ldots, \boldsymbol{X}_K \boldsymbol{M}_K\}\right), \quad \text{with } \boldsymbol{M}_k^T \boldsymbol{M}_k = \boldsymbol{I}_{r_k},\ \boldsymbol{M}_k \in \mathbb{R}^{p_k \times r_k} \quad \text{for all } k = 1, \ldots, K. \tag{1}$$

where $\mathcal{C} \in \mathbb{R}^{r_1 \times \cdots \times r_K}$ is a full-rank core tensor, ~~and~~ $\boldsymbol{M}_k \in \mathbb{R}^{p_k \times r_k}$ are factor matrices consisting of orthonormal columns ~~, where~~ with $r_k \leq p_k$ for all $k \in [K]$, and $f(\cdot)$ is a known link function whose form depending on the data type of $\mathcal{Y}$. Common choices of link functions include identity link for Gaussian distribution, logistic link for Bernoulli distribution, and $\exp(\cdot)$ link for Poisson distribution.

Figure 1b provides a schematic illustration of our model. The features $\boldsymbol{X}_k$ affect the distribution of tensor entries in $\mathcal{Y}$ through the form $\boldsymbol{X}_k \boldsymbol{M}_k$, which are r_k linear combinations of features on mode k. The core tensor $\mathcal{C}$ collects the interaction effects between sufficient features across K modes, which links the conditional mean to the feature spaces, and thereby allows the identification of variations in the tensor data attributable to the side information. Our goal is to find $\boldsymbol{M}_k$ and the corresponding $\mathcal{C}$, thereby allowing us to reveal the relationship between side information $\boldsymbol{X}_k$ and the observed tensor $\mathcal{Y}$. Note that $\boldsymbol{M}_k$ and $\mathcal{C}$ are identifiable only up to orthonormal transformations.

We give two examples of supervised tensor decomposition models (1) that arise in practice.

Example 1 (Spatio-temporal growth model)**.** The growth curve model (Srivastava et al., 2008) was originally proposed as an example of bilinear model for matrix data, and we extend it to higher-order cases. Let $\mathcal{Y} = [\![y_{ijk}]\!] \in \mathbb{R}^{d \times m \times n}$ denote the pH measurements of d lakes at m levels of depth and for n time points. Suppose the sampled lakes belong to q types, with p lakes in each type. Let $\{\ell_j\}_{j \in [m]}$ denote the sampled depth levels and $\{t_k\}_{k \in [n]}$ the time points. Assume that the expected pH trend in depth is a polynomial of order at most r and that the expected trend in time is a polynomial of order s. Then, the conditional mean model for the spatio-temporal growth is a special case of our

model (1), where $\boldsymbol{X}_1 = \text{blockdiag}\{\mathbf{1}_q, \ldots, \mathbf{1}_q\} \in \{0,1\}^{d \times p}$ is the design matrix for lake types,

$$\boldsymbol{X}_2 = \begin{pmatrix} 1 & \ell_1 & \cdots & \ell_1^r \\ 1 & \ell_2 & \cdots & \ell_2^r \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \ell_m & \cdots & \ell_m^r \end{pmatrix}, \ \boldsymbol{X}_3 = \begin{pmatrix} 1 & t_1 & \cdots & t_1^s \\ 1 & t_2 & \cdots & t_2^s \\ \vdots & \vdots & \ddots & \vdots \\ 1 & t_n & \cdots & t_n^s \end{pmatrix}$$

are the design matrices for spatial and temporal effects, respectively. The spatial-temporal mode has covariates available on each of the three modes.

Example 2 (Network population model)**.** Network response model is recently developed in the context of neuroimanig analysis. The goal is to study the relationship between network-valued response and the individual covariates. Suppose we observe n i.i.d. observations $\{(\boldsymbol{Y}_i, \boldsymbol{x}_i) : i = 1, \ldots, n\}$, where $\boldsymbol{Y}_i \in \{0,1\}^{d \times d}$ is the brain connectivity network on the i-th individual, and $\boldsymbol{x}_i \in \mathbb{R}^p$ is the individual covariate such as age, gender, cognition, etc. The network-response model (Rabusseau and Kadri, 2016) has the form

$$\text{logit}(\mathbb{E}(\boldsymbol{Y}_i | \boldsymbol{x}_i)) = \mathcal{B} \times_3 \boldsymbol{x}_i, \quad \text{for } i = 1, \ldots, n \tag{2}$$

where $\mathcal{B} \in \mathbb{R}^{d \times d \times p}$ is the coefficient tensor of interest. The model (2) is also a special case of our tensor-response model, with covariates on the last mode of the tensor.

3 Estimation algorithms

We develop a likelihood-based procedure to estimate $\mathcal{C}$ and $\boldsymbol{M}_k$ in (1). Ignoring constants that do not depend on Θ, the quasi log-likelihood of (1) is equal to

$$\mathcal{L}_{\mathcal{Y}}(\mathcal{C}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_K) = \langle \mathcal{Y}, \Theta \rangle - \sum\nolimits_{i_1, \ldots, i_K} b(\theta_{i_1, \ldots, i_K}) \text{ with } \Theta = \mathcal{C} \times \{\boldsymbol{M}_1 \boldsymbol{X}_1, \ldots, \boldsymbol{M}_K \boldsymbol{X}_K\},$$

where $b(\theta) = \theta^2/2$ for Gaussian response, $b(\theta) = \exp(\theta)$ for Poisson response, and $b(\theta) = \log(1 + \exp(\theta))$ for Bernoulli response. We propose a constrained maximum quasi-likelihood estimator (M-estimator),

$$(\hat{\mathcal{C}}, \hat{\boldsymbol{M}}_1, \ldots, \hat{\boldsymbol{M}}_k) = \underset{(\mathcal{C}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_K) \in \mathcal{P}}{\arg\max} \mathcal{L}_{\mathcal{Y}}(\mathcal{C}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_K), \tag{3}$$

where parameter space $\mathcal{P} = \left\{ (\mathcal{C}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_K) \;\middle|\; \boldsymbol{M}_k^T \boldsymbol{M}_k = \mathbf{I}_{r_k}, \ \|\Theta(\mathcal{C}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_K)\|_\infty \le \alpha \right\}$.

The decision variables in the objective function (3) consist of $K + 1$ blocks of variables, one for the core tensor $\mathcal{C}$ and K for the factor matrices $\boldsymbol{M}_k$. We notice that, if any K out of the $K + 1$ blocks of variables are known, then the optimization reduces to a simple GLM with respect to the last block of variables. This observation leads to an iterative updating scheme for one block at a time while keeping others fixed. A simplified version of the algorithm is described in Algorithm 1.

Algorithm 1 Supervised Tensor Decomposition with Interactive Side Information (Simplified)

Input: Response tensor $\mathcal{Y} \in \mathbb{R}^{d_1 \times \cdots \times d_K}$, feature matrices $\boldsymbol{X}_k \in \mathbb{R}^{d_k \times p_k}$ for $k = 1, \ldots, K$, target Tucker rank $\boldsymbol{r} = (r_1, \ldots, r_K)$, link function f, maximum norm bound α

Output: Estimated core tensor $\hat{\mathcal{C}} \in \mathbb{R}^{r_1 \times \cdots \times r_K}$ and factor matrices $\hat{\boldsymbol{M}}_k \in \mathbb{R}^{p_k \times r_k}$.

1: Random initialization of the core tensor $\mathcal{C}$ and factor matrices $\boldsymbol{M}_k$.
2: **while** Do until convergence **do**
3: Obtain $\tilde{\boldsymbol{M}}_k \in \mathbb{R}^{p_k \times r_k}$ by a GLM. Orthogonalize $\tilde{\boldsymbol{M}}_k$ by QR factorization, for $k \in [K]$.
4: Update the core tensor $\mathcal{C}$ by solving a GLM. Rescale the core tensor $\mathcal{C}$ such that $\|\mathcal{C}\|_{\max} \le \alpha$.
5: **end while**

We provide the accuracy guarantee for the proposed M-estimator (3) by leveraging recent development in random tensor theory and high-dimensional statistics.

Theorem 3.1 (Convergence)**.** Let $(\hat{\mathcal{C}}, \hat{\boldsymbol{M}}_1, \ldots, \hat{\boldsymbol{M}}_K)$ be the M-estimator in (3) and $\hat{\mathcal{B}} = \hat{\mathcal{C}} \times \hat{\boldsymbol{M}}_1 \times \cdots \times \hat{\boldsymbol{M}}_K$. Define $r_{\text{total}} = \prod_k r_k$ and $r_{\max} = \max_k r_k$. Under mild technical assumptions, there exist two positive constants $C_1, C_2 > 0$, such that, with probability at least $1 - \exp(-C_1 \sum_k p_k)$,

$$\|\mathcal{B}_{\text{true}} - \hat{\mathcal{B}}\|_F^2 \le \frac{C_2 r_{\text{total}}}{r_{\max}} \frac{\sum_k p_k}{\prod_k d_k}, \quad \text{and} \quad \sin^2 \Theta(\boldsymbol{M}_{k,\text{true}}, \hat{\boldsymbol{M}}_k) \le \frac{C_2 r_{\text{total}}}{r_{\max} \sigma_{\min}^2(\text{Unfold}_k(\mathcal{C}_{\text{true}}))} \frac{\sum_k p_k}{\prod_k d_k},$$

where $\sin \Theta(\boldsymbol{M}_{k,\text{true}}, \hat{\boldsymbol{M}}_k) = \|\boldsymbol{M}_{k,\text{true}}^T \hat{\boldsymbol{M}}_k^\perp\|_\sigma$ is the angle distance between column spaces.

Theorem 3.1 implies that the estimation has a convergence rate $\mathcal{O}(d^{-(K-1)})$ in the special case when tensor dimensions are equal on each of the modes, i.e., $d_k = d$ for all $k \in [K]$, and feature dimension grows with tensor dimension, $p_k = \gamma d$, $\gamma \in [0, 1)$, for $k \in [K]$. The convergence of our estimation becomes especially favorable as the order of tensor data increases.

4 Numerical experiments

We compare our supervised tensor decomposition (**STD**) with three other supervised tensor methods: Higher-order low-rank regression (**HOLRR** Rabusseau and Kadri (2016)), Higher-order partial least square (**HOPLS** Zhao et al. (2012)) and Subsampled tensor projected gradient (**TPG** Yu and Liu (2016)). Figure 2 shows that **STD** outperforms others, especially in the low-signal, high-rank setting. As the number of informative modes (i.e., modes with available features) increases, the **STD** exhibits a substantial reduction in error whereas others remain unchanged (Figure 2b). This showcases the benefit of incorporation of multiple features. The accuracy gain in Figure 2 demonstrates the benefit of alternating algorithm – incorporation of informative modes also improves the estimation in the non-informative modes.

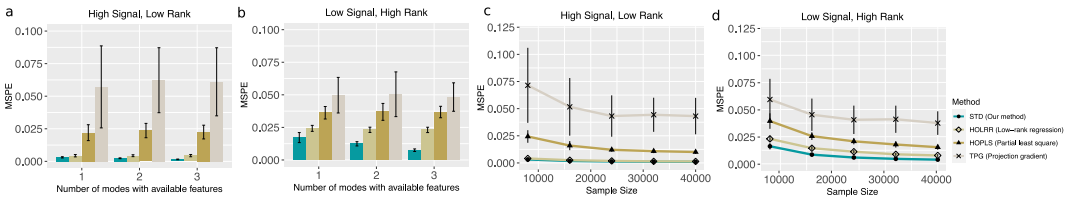

Figure 2: Comparison between different tensor methods. Panels (a) and (b) plot mean squared prediction error (MSPE) versus the number of modes with available features. Panels (c) and (d) plot MSPE versus the effective sample size d^2. We consider rank $\boldsymbol{r} = (3, 3, 3)$ (low) vs (4,5,6) (high), and signal $\alpha = 3$ (low) vs. 6 (high).

We then apply our method to brain structural connectivity networks from Human Connectome Project (HCP) (Geddes, 2016). The dataset consists of 136 brain structural networks, one for each individual. Each brain network is represented as a 68-by-68 binary matrix, where the entries encode the presence or absence of fiber connections between the 68 brain regions. We consider four individual features: gender (65 females vs. 71 males), age 22-25 ($n = 35$), age 26-30 ($n = 58$), and age 31+ ($n = 43$). The goal is to identify the connection edges that are affected by individual features.

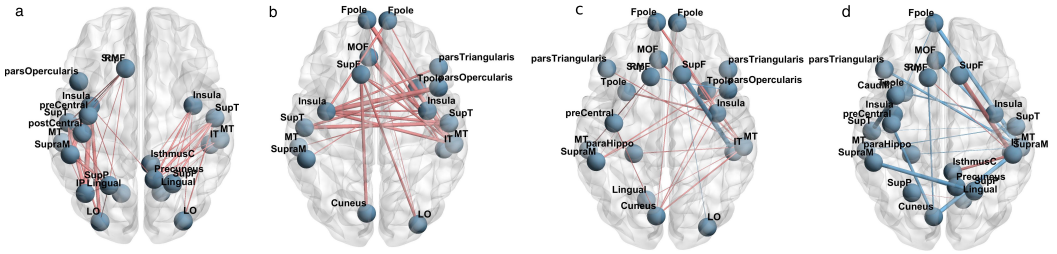

Figure 3: Top edges with large effects. (a) Global effect; (b) Female effect; (c) Age 22-25; (d) Age 31+. Red (blue) edges represent positive (negative) effects. Edge-widths are proportional to the magnitudes of effect sizes.

We perform the supervised tensor decomposition to the HCP data. The BIC selection suggests a rank $\boldsymbol{r} = (10, 10, 4)$ with quasi log-likelihood $\mathcal{L}_{\mathcal{Y}} = -174654.7$. Figure 3 shows the top edges with high effect size, overlaid on the Desikan atlas brain template (Desikan et al., 2006). We find that the global connection exhibits clear spatial separation, and that the nodes within each hemisphere are more densely connected with each other (Figure 3a). In particular, the superior-temproal (*SupT*), middle-temporal (*MT*) and Insula are the top three popular nodes in the network. Interestingly, female brains display higher inter-hemispheric connectivity, especially in the frontal, parental and temporal lobes (Figure 3b). This is in agreement with a recent study showing that female brains are optimized for inter-hemispheric communication (Ingalhalikar et al., 2014). We find several edges with declined connection in the group Age 31+. Those edges involve Frontal-pole (*Fploe*), superior-frontal (*SupF*) and Cuneus nodes. Our results highlight the importance of Frontal-pole region, and the detected decline further suggests the age effects to brain connections.

5 Conclusion

We have developed a supervised tensor decomposition method with side information on multiple modes. The empirical results demonstrate the improved interpretability and accuracy over previous approaches. Applications to the brain connection data yield conclusions with sensible interpretations, suggesting the practical utility of the proposed approach.

Broader Impact

Our supervised tensor decomposition method is widely applicable to network analysis, dyadic data analysis, spatial-temporal model, and recommendation systems. We have shown the improved predictive power and enhanced interpretability by incorporating the interactive side information in tensor decomposition method. The application to the brain connection dataset yields conclusions with sensible interpretations, suggesting the practical utility of the proposed approach. Tensor learning is a clear challenge for further research. We believe that our model enriches the research of tensor-based learning and is a powerful tool to boost scientific discoveries in various fields. We hope the work opens up new inquiry that allows more machine learning researchers to contribute to this field.

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