

Fast Bayesian Tensor Factorization with Empirically Estimated Factors

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I am proposing a computationally efficient Bayesian tensor factorization. This is a special Tucker decomposition with factors fixed on empirically estimated/chosen values. The empirical estimates can be viewed as quick approximation to the “ideal” basis associated to a core tensor of lowest rank, highest sparsity or very simple structure (e.g. diagonal). With the imperfection, the core would be less parsimonious, but still remain sparse and low rank.

Although a constraint is applied on the factors, the flexibility of the tensor model is unscathed, when the factors contain the basis of the original tensor. Taking advantage of the sparsity in the core, a multi-way Dirichlet shrinkage prior is assigned to the scales of the core parameters, effectively reducing the core to small size.

To facilitate parallel computing and good posterior mixing, I choose empirical factors residing on Stiefel manifold. This induces conditional independence on the core parameters and allow efficient block sampling.

This method has a potential wide range of applications. For example, one could pre-assign Fourier basis as an empirical factor for high-dimension multivariate spatial tensor, and treat the core tensor as a non-parameteric estimate of spectrum. In this report, I focus on a dimension reduction application over a group of large binary adjacency matrices. I fix the empirical factor to be the bases from singular value decomposition (SVD) applied on the mean graph, inducing a low-rank and near-diagonal plane in the 3-way core.

1 Motivating Application: Dimension Reduction of a Group of Large Adjacency Matrices

Consider a three-way binary tensor $A \in \{0, 1\}^{n \times n \times m}$. This tensor is a compilation of m subjects’ connectome graphs, and each graph is a symmetric $n \times n$ binary matrix describing the connectivity among the n vertices. Let $A_{i,jk}$ denote the connectivity between vertices j and k in the i th adjacency matrix A_i .

The motivating application is to obtain a collection of low dimensional representation of the adjacency matrix for each subject, preserving most of the across-subject difference. For one matrix, SVD is routinely used to produce a diagonal vector, which is commonly low rank. For multiple matrices, it is natural to consider its extension to a *joint diagonalization*.

$$A_{i,jk} \sim \text{Bernoulli}(\Phi(\psi_{i,jk})),$$

$$\psi_{i,jk} = \sum_{r=1}^{\kappa} d_{i,r} u_{j,r} u_{k,r}, \quad (1)$$

$$\Psi_i = \{u_j^T D_i u_k\}_{j,k} = U^T D_i U$$

for $i = 1, \dots, m$, $j = 2, \dots, n$, $k = 1, \dots, (j-1)$ and $\psi_{i,jk} = \psi_{i,kj}$; $\Phi(\cdot)$ is the standard normal cumulative probability, $u_{(\cdot)}$ and $d_{(\cdot)}$ are scalars; κ is the rank of this decomposition; $D_i = \text{diag}\{d_{i,1}, \dots, d_{i,\kappa}\}$, $u_j = \{u_{j,1}, \dots, u_{j,\kappa}\}'$ is a vector and $U = [u_1 || \dots || u_n]$ is the corresponding $\kappa \times n$ matrix. Since the diagonal element $A_{i,jj}$ is not defined on the graph, we treat $\psi_{i,jj} = \sum_{r=1}^{\kappa} d_{i,r} u_{j,r} u_{j,r}$ as a latent variable.

The set of diagonal vectors in $\{D_i\}_{i=1,\dots,m}$ can then be used to represent the full adjacency matrices. This model is in fact a reparameterization of a parallel factor analysis (PARAFAC) decomposition. Letting $d_{i,r} = \lambda_r d_{i,r}^*$, a rank- κ PARAFAC can be obtained:

$$\psi_{i,jk} = \sum_{r=1}^{\kappa} \lambda_r d_{i,r}^* u_{j,r} u_{k,r}. \quad (2)$$

Although this is a widely used model, it suffers from the computational bottleneck related to PARAFAC. Optimization of PARAFAC is non-convex. The factors are generally non-identifiable due to permutation, scaling and rotation. To ensure local convergence, one needs carefully control the scale, which is often difficult. The rank κ is undetermined. Most importantly, for Bayesian modeling, the posterior estimation is expensive. Although it is possible to induce posterior closed-form in the full conditional distribution (e.g. with normal prior prescribed for all parameters, each row of U is conditionally normal given the others), updating one vector at a time quickly leads to slow mixing.

2 Proposed Model in Application

PARAFAC can be viewed as a special Tucker decomposition with core with non-zero value on its super-diagonal. The general Tucker without this constraint enjoys more flexibility and often lower rank (by rank, I meant the sum of modes in the core tensor).

For the same three-way tensor, first consider a a Tucker decomposition:

$$A_{i,jk} \sim \text{Bernoulli}(\Phi(\psi_{i,jk})),$$

$$\psi_{i,jk} = \sum_{r_1=1}^{\kappa} \sum_{r_2=1}^{\kappa} \sum_{r_3=1}^{\gamma} \tilde{d}_{r_1,r_2,r_3}^* u_{j,r_1} u_{k,r_2} v_{i,r_3}, \quad (3)$$

where $\{d_{r_1, r_2, r_3}^*\}_{r_1, r_2, r_3}$ form a $\kappa \times \kappa \times \gamma$ core tensor; the first and second factors are the same $\{u_{j, r_1}\}_{r_1, j}$ as a $\kappa \times n$ factor matrix, and the third factor is $\{v_{i, r_3}\}_{r_3, i}$ as a $\gamma \times m$ factor matrix.

Similar to the PARAFAC decomposition, this decomposition is reparameterized to represent the m matrices. Letting $\tilde{d}_{r_1, r_2, i} = \sum_{r_3=1}^{\gamma} \tilde{d}_{r_1, r_2, r_3}^* v_{i, r_3}$, it becomes a new core of size $\kappa \times \kappa \times m$. Using $\tilde{D}_i = \{\tilde{d}_{r_1, r_2, i}\}_{r_1, r_2}$ to denote the i th $\kappa \times \kappa$ matrix, the decomposition has similar form as (1), except now \tilde{D}_i is no long diagonal:

$$\Psi_i = \{u_j^T \tilde{D}_i u_k\}_{j, k} = U^T \tilde{D}_i U \quad (4)$$

where U and u_j are defined in the same way as in (1). One can assign prior on each array and then sample the posterior. However, this model also suffers from the non-identifiability issue due to scaling and rotation, as well as the computational inefficiency.

2.1 Factor-Constrained Tucker Decomposition

I now consider a restricted Tucker model. The first restriction is that U should reside in the Stiefel manifold $\mathcal{V}^{\kappa \times n}$, that is $UU^T = I_{\kappa}$. This constraint not only solves the scale confounding issue, but also significantly simplifies the posterior distribution for \tilde{D}_i . Using prior $d_{i, jk} \sim N(0, \tau_{jk})$, the posterior can be sampled in a block for all index over i, j, k :

$$\begin{aligned} \tilde{d}_{i, jk} &\sim \text{No}\left\{\left(\frac{1}{2} + \frac{1}{\tau_{i, jk}}\right)^{-1} \frac{(UZ_i U^T)_{jk}}{2}, \left(\frac{1}{2} + \frac{1}{\tau_{i, jk}}\right)^{-1}\right\} \text{ for } j < k, \\ \tilde{d}_{i, kj} &= \tilde{d}_{i, jk}, \\ \tilde{d}_{i, jj} &\sim \text{No}\left\{\left(1 + \frac{1}{\tau_{i, jj}}\right)^{-1} (UZ_i U^T)_{jj}, \left(1 + \frac{1}{\tau_{i, jj}}\right)^{-1}\right\}, \end{aligned} \quad (5)$$

where $(UZ_i U^T)_{jk}$ denotes the (j, k) th element in the matrix product $UZ_i U^T$, which can be computed in parallel over $i = 1, \dots, m$. And Z_i is the symmetric latent variable matrix (cites Albert-Chib):

$$\begin{aligned} z_{i, jk} &\sim \begin{cases} \text{No}_{(0, \infty)}(u_j^T \tilde{D}_i u_k, 1) & \text{if } A_{i, jk} = 1 \\ \text{No}_{(-\infty, 0)}(u_j^T \tilde{D}_i u_k, 1) & \text{if } A_{i, jk} = 0 \end{cases} \text{ for } j < k, \\ z_{i, kj} &= z_{i, jk}, \\ z_{i, jj} &\sim \text{No}(u_j^T \tilde{D}_i u_j, 2). \end{aligned} \quad (6)$$

The estimation of the factor U is difficult. When $m = 1$, U follows a Bingham-von Mises-Fisher distribution (cites Hoff 2007), but when $m > 1$ it lacks closed-form.

Instead of sampling U , I now set it to be a fixed \hat{U} and empirically estimate this matrix before sampling. I use the eigenvectors (*e.v.*) of the normal quantile of the mean adjacency matrix, *e.v.* $(\Phi^{-1}(\bar{A}))$ with $\bar{A} =$

$\frac{1}{m} \sum_i A_i$. As a basis to *diagonalize* the mean graph, empirically, it would make each slice of the core, \tilde{D}_i , in the neighborhood of a diagonal matrix, encouraging sparsity in \tilde{D}_i .

One may be concerned that the flexibility is impacted by constraining U . However, when \hat{U} is square with $\kappa = n$, it forms a linear span for any $\Psi_i \in \mathbb{R}^{n \times n}$, allowing a fully flexible model for Ψ_i . Specifically, for any symmetric matrix, letting its singular value decomposition be $\ddot{U}^T \ddot{D}_i \ddot{U}$, it can be viewed as:

$$\Psi_i = \ddot{U}^T \ddot{D}_i \ddot{U} = \hat{U}^T R \ddot{D}_i R^T \hat{U} \quad (7)$$

where $R = \hat{U} \ddot{U}^T$ is a rotation matrix and we recover $\tilde{D}_i = R \ddot{D}_i R^T$. Therefore, estimating \tilde{D}_i under the factor-constraint model would be equivalent to the one under unconstrained model.

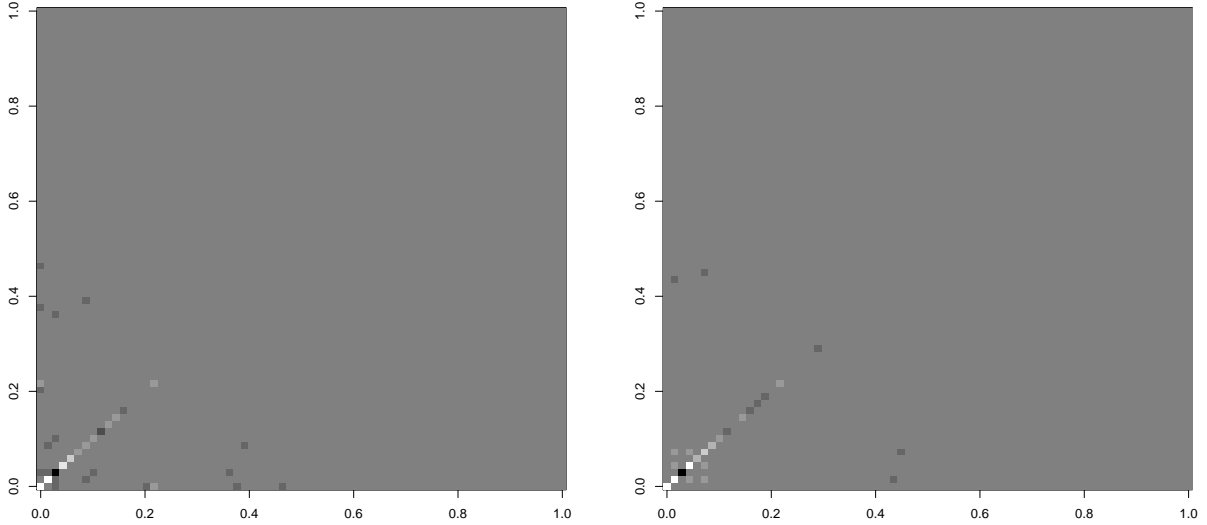


Figure 1: Estimated \tilde{D}_i for 2 random subjects showing that the empirically chosen factor induces high sparsity. Gray dots are the elements with value close to 0, while white dots are far from 0.

As an illustration, I use $m = 200$ adjacency matrices, each of size 70×70 and a weakly informative prior $\tau_{i,jk} = 1000$ for all $\tilde{D}_{i,jk}$. In order to demonstrate that the empirical factor induces a low-rank and near-diagonal core, I set the core to be full rank and this prior to temporarily not enforcing any structure (e.g. sparsity, low rank, etc) as a-priori. The posterior of \tilde{D}_i is plotted in Figure 1. High sparsity can be observed and each D_i seems to be very close to a low-rank diagonal matrix.

2.2 Shrinkage on the Scale of D_i

Setting each factor to be square requires a full-rank parameterization of $\tilde{D}_{i,jk}$, but due to the sparsity, it can be significantly simplified. Therefore, I assign a shrinkage prior on $\tau_{i,jk}$ to effectively reduce most of

parameters in $\tilde{D}_{i,jk}$ to be close to 0.

$$\begin{aligned}
\tau_{i,jk} &= \lambda_j^{(1)} \lambda_k^{(1)} \gamma_{jk} \tau_0 \quad i = 1, \dots, m, \\
\gamma_{j,k} &\sim g, \quad \tau_0 \sim f, \\
(\lambda_1^{(1)}, \dots, \lambda_n^{(1)}) &\sim \text{Dirichlet}(\alpha_1, \dots, \alpha_1)
\end{aligned} \tag{8}$$

Since the aim of this application is to obtain an equal-dimension low dimensional array for each subject, I let $\tau_{i,jk}$ to be the same for all i ; the product of $\lambda_j^{(1)} \lambda_k^{(1)}$ ensures the shrinkage is applied symmetrically in each \tilde{D}_i ; g is a heavy-tail distribution such as Laplace to allow large signal. When the tensor is of higher order p and non-symmetric, the following can be used:

$$\begin{aligned}
\tau_{i,j_1 \dots j_p} &= \lambda_{j_1}^{(1)} \lambda_{j_2}^{(2)} \dots \lambda_{j_p}^{(p)} \gamma_{j_1 \dots j_p} \tau_0 \\
\gamma_{j_1 \dots j_p} &\sim g, \quad \tau_0 \sim f, \\
(\lambda_1^{(1)}, \dots, \lambda_{n_1}^{(1)}) &\sim \text{Dirichlet}(\alpha_1, \dots, \alpha_1) \\
&\vdots \\
(\lambda_1^{(p)}, \dots, \lambda_{n_p}^{(p)}) &\sim \text{Dirichlet}(\alpha_p, \dots, \alpha_p)
\end{aligned} \tag{9}$$