

Technical Description of Dirichlet Tucker Decomposition

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1 Model

Let $\mathcal{X} \in \mathbb{N}^{M \times N \times P \times S}$ denote a four-dimensional tensor of non-negative counts $x_{m,n,p,s}$ for each mouse $m = 1, \dots, M$, epoch $n = 1, \dots, N$, position bin $p = 1, \dots, P$, and behavioral syllable $s = 1, \dots, S$. Since there are a fixed number of frames of video, C , for each mouse m and epoch n (i.e., since all epochs are the same length), the faces of the tensor, $\mathbf{X}_{m,n} = [[x_{m,n,p,s}]] \in \mathbb{N}^{P \times S}$ have a fixed sum,

$$\sum_{p=1}^P \sum_{s=1}^S x_{m,n,p,s} = C \quad \forall m, n.$$

We propose a non-negative tensor decomposition that respects this constraint.

First, define the following model parameters. Let,

- $\boldsymbol{\psi}_m \in \Delta_{K_M}$ denote the m -th **mouse loading**,
- $\boldsymbol{\phi}_n \in \Delta_{K_N}$ denote the n -th **epoch loading**,
- $\boldsymbol{\theta}_k \in \Delta_P$ for $k = 1, \dots, K_P$ denote the k -th **position factor**,
- $\boldsymbol{\lambda}_\ell \in \Delta_S$ for $\ell = 1, \dots, K_S$ denote the ℓ -th **syllable factor**, and
- $\mathcal{G} \in \mathbb{R}_+^{K_M \times K_N \times K_P \times K_S}$ denote the **core tensor** with entries $g_{i,j,k,\ell}$ and faces $\mathbf{G}_{i,j} = [[g_{i,j,k,\ell}]] \in \mathbb{R}_+^{K_P \times K_S}$.

In our model, the faces of the core tensor must be normalized such that,

$$\sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} = 1 \tag{1}$$

for all $i = 1 \dots, K_M$ and $j = 1, \dots, K_N$.

We model the data as realizations of a multinomial distribution,

$$\text{vec}(\mathbf{X}_{m,n}) \sim \text{Mult} \left(C, \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \boldsymbol{\psi}_{m,i} \boldsymbol{\phi}_{n,j} \text{vec}(\boldsymbol{\theta}_k \boldsymbol{\lambda}_\ell^\top) \right). \tag{2}$$

To check that the multinomial parameter is properly normalized, note that,

$$\begin{aligned}
\sum_{p=1}^P \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s} &= \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \left(\sum_{p=1}^P \theta_{k,p} \right) \left(\sum_{s=1}^S \lambda_{\ell,s} \right) \\
&= \sum_{i=1}^{K_M} \psi_{m,i} \sum_{j=1}^{K_N} \phi_{n,j} \left(\sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \right) \\
&= \sum_{i=1}^{K_M} \psi_{m,i} \sum_{j=1}^{K_N} \phi_{n,j} \\
&= 1,
\end{aligned}$$

where the third line follows from the assumption in eq. (1).

Prior Distributions: We place Dirichlet priors on the parameters,¹

$$\begin{aligned}
\psi_m &\stackrel{\text{iid}}{\sim} \text{Dir}(\alpha_\psi \mathbf{1}_{K_M}) \\
\phi_n &\stackrel{\text{iid}}{\sim} \text{Dir}(\alpha_\phi \mathbf{1}_{K_N}) \\
\theta_k &\stackrel{\text{iid}}{\sim} \text{Dir}(\alpha_\theta \mathbf{1}_P) \\
\lambda_\ell &\stackrel{\text{iid}}{\sim} \text{Dir}(\alpha_\theta \mathbf{1}_S) \\
\text{vec}(\mathbf{G}_{i,j}) &\stackrel{\text{iid}}{\sim} \text{Dir}(\alpha_g \mathbf{1}_{K_P \cdot K_S}).
\end{aligned}$$

The EM algorithm described below requires $\alpha > 1$. In practice, we set $\alpha_\star = 1.1$ for all parameters.

1.1 Connection to Tucker Decompositions

Under this model,

$$\mathbb{E}[x_{m,n,p,s}] = C \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}$$

More compactly,

$$\mathbb{E}[\mathcal{X}] = C \cdot \mathcal{G} \circ \Psi \circ \Phi \circ \Theta \circ \Lambda,$$

where $\Psi \in \mathbb{R}_+^{M \times K_M}$ is a matrix with rows ψ_m , $\Phi \in \mathbb{R}_+^{N \times K_N}$ is a matrix with rows ϕ_n , $\Theta \in \mathbb{R}_+^{P \times K_P}$ is a matrix with columns θ_k , $\Lambda \in \mathbb{R}_+^{S \times K_S}$ is a matrix with columns λ_ℓ , and \circ denotes a tensor-matrix multiplication. We recognize this as a 4-dimensional Tucker decomposition [Kolda and Bader, 2009] with non-negativity and normalization constraints on the factors enforced by Dirichlet priors. Hence, we call this model a **Dirichlet Tucker Decomposition**.

¹ Δ_K denotes the $(K-1)$ -dimensional probability simplex embedded in \mathbb{R}^K .

1.2 Data Augmentation

To facilitate parameter inference, we augment the model by leveraging the Poisson/multinomial relationship.

$$x_{m,n,p,s} \sim \text{Po} \left(\sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s} \right)$$

$$\Rightarrow \text{vec}(X_{m,n}) \mid (\mathbf{1}^\top X_{m,n} \mathbf{1} = C) \sim \text{Mult} \left(C, \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \text{vec}(\theta_k \lambda_\ell^\top) \right)$$

We can “thin” the Poisson counts into those arising from each of the terms in the sum,

$$z_{m,n,p,s,i,j,k,\ell} \stackrel{\text{ind}}{\sim} \text{Po}(g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s})$$

$$\Rightarrow x_{m,n,p,s} = \left(\sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell} \right) \sim \text{Po} \left(\sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s} \right)$$

These relationships permit us to think of the multinomial observation model as arising from a sum of independent Poisson counts, conditioned on the total count summing to C .

We augment the model with a tensor of latent counts, $\mathcal{Z} \in \mathbb{N}^{M \times N \times P \times S \times K_M \times K_N \times K_P \times K_S}$, with entries $z_{m,n,p,s,i,j,k,\ell}$ defined above. In the augmented model, the complete data log likelihood is,

$$p(\mathcal{X}, \mathcal{Z} \mid \mathcal{G}, \Psi, \Phi, \Theta, \Lambda) = \prod_{m=1}^M \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \mathbb{I} \left[x_{m,n,p,s} = \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell} \right]$$

$$\prod_{m=1}^M \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \prod_{i=1}^{K_M} \prod_{j=1}^{K_N} \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} \text{Po}(z_{m,n,p,s,i,j,k,\ell} \mid g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s})$$

The key idea is that in the augmented model, the parameters can be straightforwardly estimated via expectation-maximization (EM).

2 Maximum a posteriori (MAP) estimation

To estimate the model parameters, we maximize the probability in eq. (2) using the expectation-maximization (EM) algorithm. The algorithm alternates between the E- and M-steps described below.

2.1 E-step

The E-step is to compute the posterior distribution of the latent variables \mathcal{Z} ,

$$p(\mathcal{Z} \mid \mathcal{G}, \Psi, \Phi, \Theta, \mathcal{X}) = \prod_{m=1}^M \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \text{Mult}(\mathbf{z}_{m,n,p,s} \mid x_{m,n,p,s}, \boldsymbol{\pi}_{m,n,p,s})$$

where $\pi_{m,n,p,s} \in \Delta^{K_M \cdot K_N \cdot K_P \cdot K_S}$ has entries,

$$\pi_{m,n,p,s,i,j,k,\ell} = \frac{g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}}{\sum_{i'=1}^{K_M} \sum_{j'=1}^{K_N} \sum_{k'=1}^{K_P} \sum_{\ell'=1}^{K_S} g_{i',j',k',\ell'} \psi_{m,i'} \phi_{n,j'} \theta_{k',p} \lambda_{\ell',s}}$$

For the M-steps below, we only need to compute the expected value of these augmentation variables,

$$\mathbb{E}[z_{m,n,p,s,i,j,k,\ell}] = x_{m,n,p,s} \pi_{m,n,p,s,i,j,k,\ell}.$$

2.2 M-step

In the M-step, we maximize the expected log joint probability under the posterior over \mathcal{Z} . We will do so via coordinate ascent, iteratively maximizing the expected log conditional distribution for each parameter, one at a time.

M-step for ψ_m Fixing the other parameters,

$$\begin{aligned} p(\psi_m | -) &\propto \text{Dir}(\psi_m | \alpha_\psi \mathbf{1}_{K_M}) \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \prod_{i=1}^{K_M} \prod_{j=1}^{K_N} \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} \text{Po}(z_{m,n,p,s,i,j,k,\ell} | g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}) \\ &\propto \prod_{i=1}^{K_M} \psi_{m,i}^{\alpha_\psi - 1} \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \prod_{i=1}^{K_M} \prod_{j=1}^{K_N} \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} \psi_{m,i}^{z_{m,n,p,s,i,j,k,\ell}} e^{-g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}} \mathbb{I}[\psi_m \in \Delta_{K_M}] \\ &\propto \prod_{i=1}^{K_M} \psi_{m,i}^{\alpha_{m,i} - 1} \mathbb{I}[\psi_m \in \Delta_{K_M}] \\ &= \text{Dir}(\psi_m | \alpha_m) \end{aligned}$$

where

$$\alpha_{m,i} = \alpha_\psi + \sum_{n=1}^N \sum_{p=1}^P \sum_{s=1}^S \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell}$$

and $\alpha_m = (\alpha_{m,1}, \dots, \alpha_{m,K_M})^\top$. The simplification arises thanks to the normalization constraints on the data and parameters.

The M-step maximizes the expected log probability under the posterior distribution of the augmentation variables. The maximum is at the mode of a Dirichlet distribution with parameters $\mathbb{E}[\alpha_m]$,

$$\psi_{m,i}^* = \frac{\mathbb{E}[\alpha_{m,i} - 1]}{\sum_{i'=1}^{K_M} \mathbb{E}[\alpha_{m,i'} - 1]}$$

Since $\alpha_\psi > 1$, the mode is guaranteed to exist.

The updates for the other parameters follow by symmetry.

M-step for ϕ_n By symmetry,

$$p(\phi_n | -) \propto \text{Dir}(\phi_n | \alpha_n)$$

where $\alpha_n = (\alpha_{n,1}, \dots, \alpha_{n,K_N})^\top$ with,

$$\alpha_{n,j} = \alpha_\phi + \sum_{m=1}^M \sum_{p=1}^P \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{k=1}^{K_P} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell}.$$

M-step for θ_k By symmetry,

$$p(\theta_k | -) \propto \text{Dir}(\theta_k | \alpha_k)$$

where $\alpha_k = (\alpha_{k,1}, \dots, \alpha_{k,P})^\top$ with,

$$\alpha_{k,p} = \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell}.$$

M-step for λ_ℓ By symmetry,

$$p(\lambda_\ell | -) \propto \text{Dir}(\lambda_\ell | \alpha_\ell)$$

where $\alpha_\ell = (\alpha_{\ell,1}, \dots, \alpha_{\ell,S})^\top$ with,

$$\alpha_{\ell,s} = \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{p=1}^P \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{k=1}^{K_P} z_{m,n,p,s,i,j,k,\ell}.$$

M-step for $G_{i,j}$ It is less obviously symmetric, but the updates for the faces of the core tensor follow the same form.

$$\begin{aligned} p(G_{i,j} | -) &\propto \text{Dir}(\text{vec}(G_{i,j}) | \alpha_g \mathbf{1}_{K_P \cdot K_S}) \prod_{m=1}^M \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} \text{Po}(z_{m,n,p,s,i,j,k,\ell} | g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}) \\ &\propto \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} g_{i,j,k,\ell}^{\alpha_g - 1} \prod_{m=1}^M \prod_{n=1}^N \prod_{p=1}^P \prod_{s=1}^S \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} g_{i,j,k,\ell}^{z_{m,n,p,s,i,j,k,\ell}} e^{-g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}} \mathbb{I}[\text{vec}(G_{i,j}) \in \Delta_{K_P \cdot K_S}] \\ &\propto \prod_{k=1}^{K_P} \prod_{\ell=1}^{K_S} g_{i,j,k,\ell}^{\alpha_{i,j,k,\ell} - 1} \mathbb{I}[\text{vec}(G_{i,j}) \in \Delta_{K_P \cdot K_S}] \\ &= \text{Dir}(\text{vec}(G_{i,j}) | \text{vec}(A_{i,j})) \end{aligned}$$

where $A_{i,j} = [[\alpha_{i,j,k,\ell}]] \in \mathbb{R}_+^{K_P \times K_S}$ with,

$$\alpha_{i,j,k,\ell} = \alpha_g + \sum_{m=1}^M \sum_{n=1}^N \sum_{p=1}^P \sum_{s=1}^S z_{m,n,p,s,i,j,k,\ell}.$$

2.3 EM with collapsed allocation tensor

The augmented tensor of expected latent counts, $\mathcal{Z} \in \mathbb{N}^{M \times N \times P \times S \times K_M \times K_N \times K_P \times K_S}$, greatly simplifies the estimation of the model parameters, but it incurs a significant memory footprint. We note this counts allocation tensor is immediately collapsed during the M-step of each parameter, suggesting that we do not necessarily need to instantiate the tensor in its entirety during implementation.

For example, consider the M-step for θ_k . In the derivation above, we found that expected log conditional probability is maximized at the mode of the Dirichlet distribution with parameter $\mathbb{E}[\alpha_k]$ for pseudo-counts vector $\alpha_k \in \mathbb{R}_+^P$ with elements

$$\alpha_{k,p} = \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell}.$$

The expected value is,

$$\begin{aligned} \mathbb{E}[\alpha_{k,p}] &= \alpha_\theta + \mathbb{E} \left[\sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} z_{m,n,p,s,i,j,k,\ell} \right] \\ &= \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} \mathbb{E}[z_{m,n,p,s,i,j,k,\ell}] \\ &= \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} (x_{m,n,p,s} \pi_{m,n,p,s,i,j,k,\ell}) \\ &= \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \left(x_{m,n,p,s} \left(\sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} \pi_{m,n,p,s,i,j,k,\ell} \right) \right). \end{aligned}$$

Expanding the definition of $\pi_{m,n,p,s,i,j,k,\ell}$, the inner sum simplifies to

$$\sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} \pi_{m,n,p,s,i,j,k,\ell} = \frac{r_{m,n,p,s,k}}{C_{m,n,p,s}}$$

where

$$C_{m,n,p,s} = \sum_{i'=1}^{K_M} \sum_{j'=1}^{K_N} \sum_{k'=1}^{K_P} \sum_{\ell'=1}^{K_S} g_{i',j',k',\ell'} \psi_{m,i'} \phi_{n,j'} \theta_{k',p} \lambda_{\ell',s}$$

is the normalizing constant, and

$$r_{m,n,p,s,k} = \sum_{i=1}^{K_M} \sum_{j=1}^{K_N} \sum_{\ell=1}^{K_S} g_{i,j,k,\ell} \psi_{m,i} \phi_{n,j} \theta_{k,p} \lambda_{\ell,s}$$

is the collapsed allocation tensor. Given these two quantities, we can compute the expectation as,

$$\mathbb{E}[\alpha_{k,p}] = \alpha_\theta + \sum_{m=1}^M \sum_{n=1}^N \sum_{s=1}^S \left(\frac{x_{m,n,p,s} r_{m,n,p,s,k}}{C_{m,n,p,s}} \right).$$

Note that the temporary variables required for this computation use only $\mathcal{O}(MNPS)$ and $\mathcal{O}(MNPSK_P)$ memory, respectively — a dramatic reduction from the memory required to store \mathcal{Z} naively.

3 Model Selection

The main hyperparameters to be determined are the number of factors, K_M , K_N , K_P , and K_S . We choose these parameters using cross-validation using a random, speckled test set. Specifically, we hold out a random subset of faces $\mathbf{X}_{m,n}$ from the data; i.e., we mask a random subset of (mouse, epoch) pairs. That way, we still have enough observed data to estimate the mouse loadings, ψ_m , for each mouse, and the epoch loadings, ϕ_n , for each epoch. In the algorithms above, we can incorporate the mask by fixing the augmentation variables $z_{m,n,p,s,i,j,k,\ell}$ to zero whenever the index (m,n) is held out. We evaluate the log likelihood of the held out data under the multinomial model in eq. (2), using the estimated parameters.

We sweep over a four-dimensional grid of numbers of factors $K_M \in \{2, 4, \dots, 24\}$, $K_N \in \{2, 4, \dots, 8\}$, $K_P \in \{2, 4, \dots, 8\}$, and $K_S \in \{2, 4, \dots, 24\}$. The bounds of this search space were chosen manually to ensure that higher held out log likelihood could not be achieved with a larger model.

4 Implementation

We implemented this model using JAX to parallelize the updates across mice and voxels. We fit the model on an NVidia A100 GPU. The algorithm takes between 5 minutes for the smallest models and 2 hours for the largest. These ranges include the time it takes to compile the algorithm.

Our code is open source and available at <https://github.com/lindermanlab/dirichlet-tucker>.

References

T. G. Kolda and B. W. Bader. Tensor decompositions and applications. *SIAM review*, 51(3):455–500, 2009.