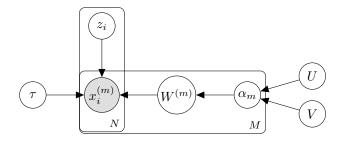
# Advanced Machine Learning, Final Project. Model Inference.

#### January 15, 2016

## Model

We begin by presenting the graphical model corresponding to group factor analysis:



Where:

 $X \in \mathbb{R}^{N \times D}$  such that:

$$\begin{split} X &= [X^{(1)},...,X^{(M)}] \\ X^{(m)\intercal} &= [x_1^{(m)},...,x_N^{(m)}] \\ p(X|W,Z,\tau) &= \prod_i \prod_m \mathcal{N}(x_i^{(m)}|W^{(m)\intercal}z_i,\tau_m^{-1}\mathbf{I}) \end{split}$$

 $\tau \in \mathbb{R}^{1 \times M}$  such that:

$$\begin{split} \tau &= [\tau_1, ..., \tau_M] \\ p(\tau) &= \prod_m \mathcal{G}(\tau_m | a^\tau = 10^{-14}, b^\tau = 10^{-14}) \end{split}$$

 $Z \in \mathbb{R}^{N \times K}$  such that:

$$Z^{\mathsf{T}} = [z_1, ..., z_N]$$
  
 $p(Z) = \prod_i \mathcal{N}(z_i | \mathbf{0}, \mathbf{1})$ 

$$W \in \mathbb{R}^{K \times D}$$
 such that:

$$\begin{split} W &= [W^{(1)}, ..., W^{(M)}] \\ W^{(m)\intercal} &= [w_1^{(m)}, ..., w_K^{(m)}] \\ w_k^{(m)} &\in \mathbb{R}^{D_m} \\ \sum_{m=1}^M D_m &= D \\ p(W|\alpha) &= \prod_{m=1}^M \prod_{k=1}^K \prod_{d=1}^{D_m} \mathcal{N}(w_{k,d}^{(m)}|0, \alpha_{m,k}^{-1}) \end{split}$$

 $\alpha \in \mathbb{R}^{M \times K}$  such that:

$$log(\alpha) = UV^{\mathsf{T}} + \mu_u \mathbf{1}^{\mathsf{T}} + \mathbf{1}\mu_v^{\mathsf{T}}.$$

 $U \in \mathbb{R}^{M \times R}$ 

$$p(U) = \prod_{m=1}^{M} \prod_{r=1}^{R} \mathcal{N}(u_{m,r}|0, (\lambda = 0.1)^{-1})$$

 $V \in \mathbb{R}^{K \times R}$ 

$$p(V) = \prod_{k=1}^{K} \prod_{r=1}^{R} \mathcal{N}(v_{k,r}|0, (\lambda = 0.1)^{-1})$$

Then the model's full joint probability can be written as:

$$p(\Theta, X) = p(Z, W, \tau, U, V, X) = p(Z)p(W|\alpha)p(\tau)p(U)p(V)p(X|W, Z, \tau)$$

#### Inference

In order to minimize the Kullback-Leibler divergence:

$$D_{KL}(q||p) = \int_{\Theta} q(\Theta)log(\frac{q(\Theta)}{p(\Theta|X)})d\Theta$$

or equivalently to maximize the lower bound:

$$\mathcal{L}(\Theta) = \int_{\Theta} q(\Theta) log(\frac{p(\Theta, X)}{q(\Theta)}) d\Theta$$

We assume:

$$q(\Theta) = q(Z)q(W)q(\tau)q(U)q(V)$$

In which case and by means of variational calculus we must have that  $q(\theta_i)$  must have the form:

$$q(\theta_i) = \frac{e^{E_{i \neq j}[log(p(\Theta, X))]}}{\int e^{E_{i \neq j}[log(p(\Theta, X))]}d\theta_i}$$

$$\implies log(q(\theta_i)) = E_{i \neq j}[log(p(\Theta, X))] + constant$$

And so we proceed by taking the corresponding expectations with respect to the log of the model's full joint probability:

$$log(q(Z)) = E_{W_{\tau}}[log(p(\Theta, X))] = E_{W_{\tau}}[log(p(Z))] + E_{W_{\tau}}[log(p(X|W, Z, \tau))] + C_1$$

$$= E_{W,\tau}\bigg[\sum_{i}^{N} log(\mathcal{N}(z_{i}|\mathbf{0},\mathbf{I}))\bigg] + E_{W,\tau}\bigg[\sum_{i}^{N}\sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}))\bigg] + C_{1}$$

$$= -\frac{1}{2} \sum_{i}^{N} z_{i}^{\mathsf{T}} z_{i} - \frac{1}{2} \sum_{m}^{M} E_{W,\tau} \bigg[ \tau_{m} (x_{i}^{(m)} - W^{(m)\mathsf{T}} z_{i})^{\mathsf{T}} (x_{i}^{(m)} - W^{(m)\mathsf{T}} z_{i}) \bigg] + C_{2}$$

$$= -\frac{1}{2} \sum_{i}^{N} z_{i}^{\mathsf{T}} \mathbf{I}_{k} z_{i} + \sum_{m}^{M} \langle \tau_{m} \rangle (z_{i}^{\mathsf{T}} \langle W^{(m)} \rangle x_{i}^{(m)} - \frac{1}{2} z_{i}^{\mathsf{T}} \langle W^{(m)} W^{(m)\mathsf{T}} \rangle z_{i}) + C_{3}$$

$$= \sum_{i}^{N} \sum_{m}^{M} z_{i}^{\mathsf{T}} \langle W^{(m)} \rangle \langle \tau_{m} \rangle x_{i}^{(m)} - \frac{1}{2} z_{i}^{\mathsf{T}} (\mathbf{I}_{k} + \sum_{m}^{M} \langle \tau_{m} \rangle \langle W^{(m)} W^{(m)\mathsf{T}} \rangle) z_{i} + C_{3}$$

Note that above we denote the first moment by  $E_{\theta_i}[\theta_i] = \langle \theta_i \rangle$  and the second moment by  $E_{\theta_i}[\theta_i \theta_i^{\mathsf{T}}] = \langle \theta_i \theta_i^{\mathsf{T}} \rangle$ . Note as well that we collect all constant factors with respect to  $z_i$  into  $C_1$ ,  $C_2$  and  $C_3$  respectively. Then recalling:

$$\mathcal{N}(x|\mu,\Sigma) \propto x^{\mathsf{T}} \Sigma^{-1} \mu - \frac{1}{2} x^{\mathsf{T}} \Sigma^{-1} x$$

We must have:

$$q(Z) = \prod_{i}^{N} \mathcal{N}(m_i^{(z)}, \Sigma^{(z)})$$

with:

$$\Sigma^{(z)} = \left(\mathbf{I}_k + \sum_{m}^{M} \langle \tau_m \rangle \langle W^{(m)} W^{(m)} \mathsf{T} \rangle \right)^{-1}$$
$$m_i^{(z)} = \Sigma^{(z)} \langle W^{(m)} \rangle \langle \tau_m \rangle x_i^{(m)}$$

Similarly we proceed with q(W) in which case we have:

$$log(q(W)) = E_{\alpha,Z,\tau}[log(p(\Theta,X))] = E_{\alpha,Z,\tau}[log(p(W|\alpha))] + E_{\alpha,Z,\tau}[log(p(X|W,Z,\tau))] + C_1$$

$$= E_{\alpha,Z,\tau} \bigg[ \sum_{m}^{M} \sum_{k}^{K} \sum_{d}^{D_{m}} log(\mathcal{N}(w_{k,d}^{(m)}|0,\alpha_{m,k}^{-1})) \bigg] + E_{\alpha,Z,\tau} \bigg[ \sum_{i}^{N} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] + C_{1} \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{K} \sum_{i}^{D_{m}} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] + C_{1} \bigg] \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{K} \sum_{i}^{D_{m}} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] + C_{1} \bigg] \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{K} \sum_{i}^{D_{m}} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] + C_{1} \bigg] \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{K} \sum_{i}^{D_{m}} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] \bigg] + C_{1} \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] \bigg] \bigg] \bigg] \bigg] \bigg] \bigg] \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] \bigg] \bigg] \bigg] \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}) \bigg] \bigg] \bigg[ \sum_{i}^{M} \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}) \bigg] \bigg] \bigg[ \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I})) \bigg] \bigg] \bigg] \bigg] \bigg[ \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}) \bigg] \bigg] \bigg[ \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}) \bigg] \bigg] \bigg] \bigg[ \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m}^{-1}\mathbf{I}) \bigg] \bigg[ \sum_{m}^{M} log(\mathcal{N}(x_{i}^{(m)}|W^{(m)\intercal}z_{i},\tau_{m$$

We continue by looking at the group columns  $w_{:,d}^{(m)}$  in W as opposed to the group rows  $w_k^{(m)}$  such that  $W^{(m)} = [w_{:,1}^{(m)},...,w_{:,D_m}^{(m)}]$ . Then note that the number of columns in X is equal to the number of columns in W and so we have:

$$=E_{\alpha,Z,\tau}\bigg[\sum_{m}^{M}\sum_{d}^{D_{m}}\log(\mathcal{N}(w_{:,d}^{(m)}|\mathbf{0},\overline{\overline{\alpha}}_{m}^{-1}))\bigg]+E_{\alpha,Z,\tau}\bigg[\sum_{m}^{M}\sum_{d}^{D_{m}}\sum_{i}^{N}\log(\mathcal{N}(x_{i,d}^{(m)}|w_{:,d}^{(m)}^{\tau}z_{i},\tau_{m}^{-1}))\bigg]+C_{1}$$

Where  $\overline{\overline{\alpha}}_m$  is the m-th row of  $\alpha$  transformed into a diagonal  $K \times K$  matrix.

$$= -E_{\alpha,Z,\tau} \left[ \frac{1}{2} \sum_{m}^{M} \sum_{d}^{D_{m}} w_{:,d}^{(m)\mathsf{T}} \overline{\overline{\alpha}}_{m} w_{:,d}^{(m)} \right] - E_{\alpha,Z,\tau} \left[ \frac{1}{2} \sum_{m}^{M} \sum_{d}^{D_{m}} \sum_{i}^{N} \tau_{m} (x_{i,d}^{(m)} - w_{:,d}^{(m)\mathsf{T}} z_{i})^{2} \right] + C_{2}$$

$$= -\frac{1}{2} \sum_{m}^{M} \sum_{i,d}^{D_{m}} w_{:,d}^{(m)\intercal} \langle \overline{\overline{\alpha}}_{m} \rangle w_{:,d}^{(m)} - \frac{1}{2} \sum_{m}^{M} \sum_{i}^{D_{m}} \sum_{j}^{N} \langle \tau_{m} \rangle (-2x_{i,d}^{(m)} w_{:,d}^{(m)\intercal} \langle z_{i} \rangle + w_{:,d}^{(m)\intercal} \langle z_{i} z_{i}^{\intercal} \rangle w_{:,d}^{(m)}) + C_{3}$$

$$=\sum_{m}^{M}\sum_{d}^{D_{m}}\left\langle \tau_{m}\right\rangle \sum_{i}^{N}w_{:,d}^{(m)\intercal}x_{i,d}^{(m)}\left\langle z_{i}\right\rangle -\frac{1}{2}\sum_{m}^{M}\sum_{d}^{D_{m}}w_{:,d}^{(m)\intercal}(\left\langle \tau_{m}\right\rangle \sum_{i}^{N}\left\langle z_{i}z_{i}^{\intercal}\right\rangle +\left\langle \overline{\overline{\alpha}}_{m}\right\rangle )w_{:,d}^{(m)}+C_{3}$$

Then again recalling that  $\mathcal{N}(x|\mu,\Sigma) \propto x^\intercal \Sigma^{-1} \mu - \frac{1}{2} x^\intercal \Sigma^{-1} x$ , we must have that  $q(W) = \prod_m^M \prod_d^{D_m} \mathcal{N}(w_{:,d}^{(m)}|m_{m,d}^{(w)}, \Sigma_m^{(w)})$  with:

$$\Sigma_{m}^{(w)} = \left( \langle \tau_{m} \rangle \sum_{i}^{N} \langle z_{i} z_{i}^{\mathsf{T}} \rangle + \langle \overline{\overline{\alpha}}_{m} \rangle \right)^{-1}$$

$$m_{m,d}^{(w)} = \Sigma_m^{(w)} \langle \tau_m \rangle \sum_{i}^{N} x_{i,d}^{(m)} \langle z_i \rangle$$

Moving on to  $q(\tau)$  we have:

$$log(q(\tau)) = E_{W,Z}[log(p(\Theta,X))] = E_{W,Z}[log(p(\tau)] + E_{W,Z}[log(p(X|W,Z,\tau)] + C_1] + C_1 + C_2 +$$

$$= E_{W\!,Z}\bigg[\sum_m^M log(\mathcal{G}(\tau_m|a^\tau,b^\tau))\bigg] + E_{W\!,Z}\bigg[\sum_i^N \sum_m^M log(\mathcal{N}(x_i^{(m)}|W^{(m)\intercal}z_i,\tau_m^{-1}\mathbf{I}))\bigg] + C_1$$

$$= E_{W,Z} \left[ \sum_{m}^{M} (a^{\tau} - 1) log(\tau_{m}) - b^{\tau} \tau_{m} \right] + E_{W,Z} \left[ -\frac{1}{2} \sum_{m}^{M} \sum_{i}^{N} log(|\tau_{m}^{-1} \mathbf{I}|) - (x_{i}^{(m)} - W^{(m)\intercal} z_{i})^{2} \tau_{m} \right] + C_{2}$$

Then notice that  $log(|\tau_m^{-1}\mathbf{I}|) = -D_m log(\tau_m)$  and so we have:

$$=\sum_{m}^{M}(a^{\tau}+\frac{ND_{m}}{2}-1)log(\tau_{m})-\left(b^{\tau}+\sum_{i}^{N}\left\langle (x_{i}^{(m)}-W^{(m)\intercal}z_{i})^{2}\right\rangle \right)\tau_{m}+C_{2}$$

Which has the form of a new Gamma distribution and thus we must have that  $q(\tau) = \prod_m^M \mathcal{G}(\tau_m | a_m^{\tau}, b_m^{\tau})$  where:

$$a_m^{\tau} = a^{\tau} + \frac{ND_m}{2}$$

$$b_m^{\tau} = b^{\tau} + \sum_{i}^{N} \left\langle (x_i^{(m)} - W^{(m)\mathsf{T}} z_i)^2 \right\rangle$$

Finally we turn our attention to U and V:

$$\mathcal{L}(\Theta) = \int_{\Theta} q(\Theta) log(\frac{p(\Theta, X)}{q(\Theta)}) d\Theta$$

$$= \int_{\Theta} q(Z,W,\tau)q(U)q(V)log(\frac{p(Z,\tau,X)p(U,V)p(W|\alpha)}{q(Z,W,\tau)q(U)q(V)})dZdWd\tau dUdV$$

If we concentrate on U and V and regard the remaining variables as constant we then have:

$$\propto \int_{UV} q(U)q(V)log(\frac{p(U,V)p(W|\alpha)}{q(U)q(V)})dUdV$$

At this point we use fixed-form distributions for q(U) and q(V) such that  $q(U) = \delta_U$  and  $q(V) = \delta_V$  and:

$$\propto \int_{UV} log(p(U,V)) + log(p(W|U,V))dUdV$$

$$= \int_{UV} log(p(U, V)) + \sum_{m}^{M} \sum_{k}^{K} \sum_{d}^{D_{m}} log(\mathcal{N}(w_{k, d}^{(m)} | 0, \alpha_{m, k}^{-1})) dU dV$$

$$= \int_{UV} log(p(U, V)) + \sum_{m}^{M} \sum_{k}^{K} \sum_{d}^{D_{m}} \frac{1}{2} log(\alpha_{m,k}) - \frac{1}{2} \alpha_{m,k} \langle w_{k,d}^{(m)2} \rangle dU dV$$

We then express  $p(W|\alpha)$  in terms of U and V as opposed to  $\alpha$ . For this recall that  $log(\alpha) = UV^{\intercal} + \mu_u + \mu_v$  but then notice that we can append both  $\mu_u$  and  $\mu_v$  to U and V respectively if we let:

$$U' = \left[ U \middle| \mu_u \middle| \mathbf{1} \right]$$

$$V' = \left\lceil V \middle| \mathbf{1} \middle| \mu_v \right\rceil$$

Such that  $log(\alpha) = U'V'^{\mathsf{T}}$  then  $\alpha_{m,k} = e^{u'_m v'_k^{\mathsf{T}}}$  and notice that the sum from d to  $D_m$  of the second moments  $\langle w_{k,d}^{(m)2} \rangle$  is the entry in the k-th column and k-th row of the matrix  $\langle W^{(m)}W^{(m)\mathsf{T}} \rangle$  and thus:

$$\propto \int_{UV} 2log(p(U,V)) + \sum_{m}^{M} \sum_{k}^{K} \left( D_{m} u'_{m} v'_{k}^{\mathsf{T}} - \langle W^{(m)} W^{(m)\mathsf{T}} \rangle_{k,k} e^{u'_{m} v'_{k}^{\mathsf{T}}} \right) dU dV$$

The expression  $L = 2log(p(U,V)) + \sum_{m}^{M} \sum_{k}^{K} \left( D_{m} u'_{m} v'^{\mathsf{T}}_{k} - \langle W^{(m)} W^{(m)\mathsf{T}} \rangle_{k,k} e^{u'_{m} v'^{\mathsf{T}}_{k}} \right)$  can be maximized by gradient descent provided we compute the derivatives  $\frac{\delta L}{\delta U}, \frac{\delta L}{\delta \mu_{n}}, \frac{\delta L}{\delta V}$  and  $\frac{\delta L}{\delta \mu_{n}}$ .

We begin by looking at p(U) and p(V) respectively where:

$$p(U) = \prod_{m=1}^{M} \prod_{r=1}^{R} p(u_{mr}) = \prod_{m=1}^{M} \prod_{r=1}^{R} \mathcal{N}(u_{mr}|0,\lambda^{-1}) = \prod_{m=1}^{M} \prod_{r=1}^{R} (\frac{\lambda}{2\pi})^{\frac{1}{2}} e^{-\frac{\lambda}{2}u_{mr}^2} = (\frac{\lambda}{2\pi})^{\frac{MR}{2}} e^{-\frac{\lambda}{2}tr(U^TU)}$$

And similarly:

$$p(V) = \left(\frac{\lambda}{2\pi}\right)^{\frac{KR}{2}} e^{-\frac{\lambda}{2}tr(V^T V)}$$

And thus we can write:

$$\begin{split} 2log(p(U,V)) &= 2log(p(U)p(V)) = 2log(e^{-\frac{\lambda}{2}(tr(U^TU) + tr(V^TV))}) + R(M+K)log(\frac{\lambda}{2\pi}) \\ &= -\lambda(tr(U^TU) + tr(V^TV)) + C \end{split}$$

Such that:

$$L = \sum_{m}^{M} \sum_{k}^{K} \left( D_{m} log(\alpha_{m,k}) - \langle W^{(m)} W^{(m)\intercal} \rangle_{k,k} \alpha_{m,k} \right) - \lambda (tr(U^{T}U) + tr(V^{T}V)) + C$$

where  $\alpha = e^{(UV^T + \mu_u \mathbf{1}^T + \mathbf{1}\mu_v^T)}$ .

Expressing first term of L with matrices:

$$\sum_{m}^{M} \sum_{k}^{K} \left( D_{m} (UV^{T} + \mu_{u} \mathbf{1}^{T} + \mathbf{1} \mu_{v}^{T})_{m,k} \right) = tr \left( D\mathbf{1}^{T} (UV^{T} + \mu_{u} \mathbf{1}^{T} + \mathbf{1} \mu_{v}^{T})^{T} \right)$$
$$= tr \left( D\mathbf{1}^{T} (VU^{T} + \mathbf{1} \mu_{u}^{T} + \mu_{v} \mathbf{1}^{T}) \right)$$

Where:

$$D^{\mathsf{T}} = [D_1, ..., D_m, ..., D_M]$$

The derivatives of first term of L are:

$$\frac{\delta Tr \Big( D\mathbf{1}^T \big( VU^T + \mathbf{1}\mu_u^T + \mu_v \mathbf{1}^T \big) \Big)}{\delta U} = D\mathbf{1}^T V \qquad \frac{\delta Tr \Big( D\mathbf{1}^T \big( VU^T + \mathbf{1}\mu_u^T + \mu_v \mathbf{1}^T \big) \Big)}{\delta \mu_u} = D\mathbf{1}^T \mathbf{1}$$

$$\frac{\delta Tr\Big(D\mathbf{1}^T\big(VU^T+\mathbf{1}\boldsymbol{\mu}_u^T+\boldsymbol{\mu}_v\mathbf{1}^T\big)\Big)}{\delta V}=(D\mathbf{1}^T)^TU \qquad \frac{\delta Tr\Big(D\mathbf{1}^T\big(VU^T+\mathbf{1}\boldsymbol{\mu}_u^T+\boldsymbol{\mu}_v\mathbf{1}^T\big)\Big)}{\delta \boldsymbol{\mu}_v}=(D\mathbf{1}^T)^T\mathbf{1}$$

The derivatives of third term of L are:

$$\frac{\delta \lambda (tr(U^TU) + tr(V^TV))}{\delta U} = 2\lambda U \qquad \frac{\delta \lambda (tr(U^TU) + tr(V^TV))}{\delta V} = 2\lambda V$$

Derivative of the second term is easier to compute element-wise and then express it with matrices. Let us denote this term as

$$L_2 = \sum_{m}^{M} \sum_{k}^{K} \langle W^{(m)} W^{(m)} \mathsf{T} \rangle_{k,k} e^{(UV^T + \mu_u \mathbf{1}^T + \mathbf{1} \mu_v^T)_{m,k}} = \sum_{m}^{M} \sum_{k}^{K} \langle W^{(m)} W^{(m)} \mathsf{T} \rangle_{k,k} e^{(\sum_{i}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})}$$

Element-wise derivatives and their matrix versions of the second term:

$$\frac{\delta L_2}{\delta u_{m,r}} = \sum_{k=0}^{K} \langle W^{(m)} W^{(m)} \mathbf{T} \rangle_{k,k} e^{(\sum_{i=0}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})} v_{k,r} \qquad \frac{\delta L_2}{\delta U} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)}) V_{k,k} e^{(\sum_{i=0}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})} v_{k,r}$$

$$\frac{\delta L_2}{\delta v_{k,r}} = \sum_{m}^{M} \langle W^{(m)} W^{(m)} \mathsf{T} \rangle_{k,k} e^{(\sum_{i}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})} u_{m,r} \qquad \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T + \mathbf{1} \mu_{v}^T)})^T U_{m,r} + \frac{\delta L_2}{\delta V} = (B \circ e^{(UV^T$$

$$\frac{\delta L_2}{\delta \mu_{u,m}} = \sum_{k}^{K} \langle W^{(m)} W^{(m)\mathsf{T}} \rangle_{k,k} e^{(\sum_{i}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})} \qquad \frac{\delta L_2}{\delta \mu_{u}} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)}) \mathbf{1}$$

$$\frac{\delta L_2}{\delta \mu_{v,k}} = \sum_{m}^{M} \langle W^{(m)} W^{(m)\mathsf{T}} \rangle_{k,k} e^{(\sum_{i}^{R} u_{m,i} v_{k,i} + \mu_{u,m} + \mu_{v,k})} \qquad \frac{\delta L_2}{\delta \mu_{v}} = (B \circ e^{(UV^T + \mu_{u} \mathbf{1}^T + \mathbf{1} \mu_{v}^T)})^T \mathbf{1}$$

Where  $\circ$  stands for the Hadamard product (element-wise matrix multiplication) and B is M  $\times$  K matrix where m-th row is the main diagonal of a corresponding  $\langle W^{(m)}W^{(m)\intercal}\rangle$ , so  $B^T=[diag(\langle W^{(1)}W^{(1)\intercal}\rangle),...,diag(\langle W^{(M)}W^{(M)\intercal}\rangle)]$ .

Final gradients are:

$$\frac{\delta L}{\delta U} = AV - 2\lambda U$$
  $\frac{\delta L}{\delta \mu_n} = A\mathbf{1}$ 

$$rac{\delta L}{\delta V} = A^\intercal U - 2\lambda V \qquad rac{\delta L}{\delta \mu_n} = A^\intercal \mathbf{1}$$

Where:

$$A = D\mathbf{1}^{\mathsf{T}} - B \circ e^{(UV^T + \mu_u \mathbf{1}^T + \mathbf{1}\mu_v^T)}$$

## Full Rank Model Inference.

Recalling:

$$L = \sum_{m}^{M} \sum_{k}^{K} \left( D_{m} log(\alpha_{m,k}) - \langle W^{(m)} W^{(m)\intercal} \rangle_{k,k} \alpha_{m,k} \right) - 2\lambda (tr(U^{\intercal}U) + tr(V^{\intercal}V)) + C$$

Then assuming  $\lambda$  to be negibly small and unrestricted by U and V we have that the derivative of L with respect to  $\alpha_{m,k}$  is given by:

$$\frac{\delta L}{\delta \alpha_{m,k}} = \frac{D_m}{\alpha_{m,k}} - \langle W^{(m)} W^{(m)\intercal} \rangle_{k,k}$$

Which in turns implies that L is maximized with respect to  $\alpha_{m,k}$  whenever:

$$\alpha_{m,k} = \frac{D_m}{\langle W^{(m)}W^{(m)\mathsf{T}}\rangle_{k,k}}$$

Moreover if we perform full variational inference over  $\alpha_{m,k}$  by setting a prior such as:

$$p(\alpha_{m,k}) = \mathcal{G}(a^{\alpha}, b^{\alpha})$$

We obtain:

$$log(q(\alpha_{m,k})) = E_W[log(p(\Theta, X))] = E_W[log(p(\alpha_{m,k}))] + E_W[log(p(W|\alpha))] + C_1$$

$$= E_{W}[log(\mathcal{G}(\alpha_{m,k}|a^{\alpha},b^{\alpha}))] + E_{W}\left[\sum_{d}^{D_{m}}log(\mathcal{N}(w_{k,d}^{(m)}|0,\alpha_{m,k}^{-1}))\right] + C_{1}$$

$$= E_W[(a^{\alpha} - 1)log(\alpha_{m,k}) - b^{\alpha}\alpha_{m,k}] + E_W\left[\frac{1}{2}\sum_{d}^{D_m}log(\alpha_{m,k}) - w_{k,d}^{(m)2}\alpha_{m,k}\right] + C_2$$

Then recall that  $\langle w_{k,d}^{(m)2} \rangle$  is the entry in the k-th column and k-th row of the matrix  $\langle W^{(m)}W^{(m)\intercal} \rangle$  and we have:

$$= \left(a^{\alpha} + \frac{D_m}{2} - 1\right) log(\alpha_{m,k}) - \left(b^{\alpha} + \frac{\langle W^{(m)}W^{(m)\intercal}\rangle_{k,k}}{2}\right) \alpha_{m,k} + C_2$$

Which has the form of a Gamma distribution such that  $q(\alpha_{m,k}) = \mathcal{G}(a_{m,k}^{\alpha},b_{m,k}^{\alpha})$  with mean  $\frac{a_{m,k}^{\alpha}}{b_{m,k}^{\alpha}}$  where:

$$a_{m,k}^{\alpha} = a^{\alpha} + \frac{D_m}{2}$$

$$b_{m,k}^{\alpha} = b^{\alpha} + \frac{\langle W^{(m)}W^{(m)\mathsf{T}}\rangle_{k,k}}{2}$$

And so we notice the resemblance between the solution provided by direct optimization and full variational inference drawing  $\alpha_{m,k}$  from a gamma prior. In particular we notice that they are exactly the same whenever  $a^{\alpha} = b^{\alpha} = 0$ . We conclude that whenever the model is full rank (i.e. R = min(M, K)) the full variational inference solution can be used instead of numerically optimizing U and V.

## Algorithm

Drawing from our results above we present the final algorithm:

#### Algorithm 1 VB inference for GFA

```
1: Initialize q(W), q(Z), q(\tau), U and V.
         while not converged do
                    Check for empty factors to be removed
  3:
                  check for empty factors to be removed q(W) \leftarrow \prod_{m}^{M} \prod_{d}^{D_{m}} \mathcal{N}(w_{:,d}^{(m)} | m_{m,d}^{(w)}, \Sigma_{m}^{(w)})
q(Z) \leftarrow \prod_{i}^{N} \mathcal{N}(m_{i}^{(z)}, \Sigma^{(z)})
if full-rank GFA (R = min(M, K)) then
q(\alpha) \leftarrow \prod_{m=1}^{M} \prod_{k=1}^{K} \mathcal{G}(a_{m,k}^{\alpha}, b_{m,k}^{\alpha})
  4:
  5:
  6:
  7:
  8:
                             U, V \leftarrow argmax_{U,V}L
  9:
                             \langle \alpha \rangle \leftarrow exp(U'V'^{\mathsf{T}})
10:
                   q(\tau) \leftarrow \prod_{m}^{M} \mathcal{G}(\tau_{m} | a_{m}^{\tau}, b_{m}^{\tau})
11:
```

## Predictive inference

When using the group factor analysis for prediction, say when we observed all but the m-th group, we can train the model in the remaining M-1 groups as usual so as to obtain estimates  $Z^*$  for the hidden variables and estimate the expected value  $\langle X^{(m)}|X^{-(m)}\rangle$  by referring to the model's original relationship between observed and hidden variables namely  $X=ZW+\epsilon$  such that:

$$\langle X^{(m)}|X^{-(m)}\rangle = \langle Z^*W^{(m)}\rangle$$

Where the expected value  $\langle Z^*W^{(m)}\rangle$  is obtained with respect to the distribution  $q(W^{(m)})q(Z^*)$ .