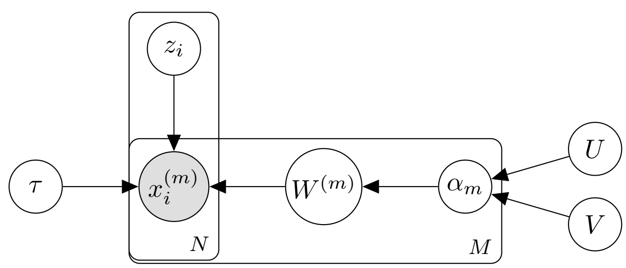
Advanced Machine Learning, Final Project.
Model Inference.

January 14, 2016

Model

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



Where:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

$$= E_{W,\tau}\left[\sum_i^N log(\mathcal{N}(z_i|\mathbf{0}, \mathbf{I}))\right] + E_{W,\tau}\left[\sum_i^N \sum_m^M log(\mathcal{N}(x_i^{(m)}|W^{(m)\intercal} z_i, \tau_m^{-1}\mathbf{I}))\right] + C_1$$

$$= -\frac{1}{2}\sum_i^N z_i^\intercal z_i - \frac{1}{2}\sum_m^M E_{W,\tau}\left[\tau_m (x_i^{(m)} - W^{(m)\intercal} z_i)^\intercal (x_i^{(m)} - W^{(m)\intercal} z_i)\right] + C_2$$

$$= -\frac{1}{2}\sum_i^N z_i^\intercal \mathbf{I}_k z_i + \sum_m^M \langle\tau_m\rangle (z_i^\intercal \langle W^{(m)}\rangle x_i^{(m)} - \frac{1}{2} z_i^\intercal \langle W^{(m)} W^{(m)\intercal}\rangle z_i) + C_3$$

$$= \sum_i^N \sum_m^M z_i^\intercal \langle W^{(m)}\rangle \langle\tau_m\rangle x_i^{(m)} - -\frac{1}{2} z_i^\intercal (\mathbf{I}_k + \sum_m^M \langle\tau_m\rangle \langle W^{(m)} W^{(m)\intercal}\rangle) z_i + C_3$$

Note that above we denote the first moment by $E_{\theta_i}[\theta_i] = \langle\theta_i\rangle$ and the second moment by $E_{\theta_i}[\theta_i\theta_i^\intercal] = \langle\theta_i\theta_i^\intercal\rangle$. 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:

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

We must have:

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

with:

$$\Sigma^{(z)} = \left(\mathbf{I}_k + \sum_m^M \langle\tau_m\rangle \langle W^{(m)} W^{(m)\intercal}\rangle\right)^{-1}$$

$$m_i^{(z)} = \Sigma^{(z)} \langle W^{(m)}\rangle \langle\tau_m\rangle x_i^{(m)}$$

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

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

$$= E_{\alpha,Z,\tau}\left[\sum_m^M \sum_k^K \sum_d^{D_m} log(\mathcal{N}(w_{k,d}^{(m)}|0, \alpha_{m,k}^{-1}))\right] + E_{\alpha,Z,\tau}\left[\sum_i^N \sum_m^M log(\mathcal{N}(x_i^{(m)}|W^{(m)\intercal} z_i, \tau_m^{-1}\mathbf{I}))\right] + C_1$$

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:

$$= E_{\alpha,Z,\tau}\left[\sum_m^M \sum_d^{D_m} log(\mathcal{N}(w_{:,d}^{(m)}|\mathbf{0}, \overline{\overline{\alpha}}_m^{-1}))\right] + E_{\alpha,Z,\tau}\left[\sum_m^M \sum_d^{D_m} \sum_i^N log(\mathcal{N}(x_{i,d}^{(m)}|w_{:,d}^{(m)\intercal} z_i, \tau_m^{-1}))\right] + C_1$$

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

$$= -E_{\alpha,Z,\tau}\left[\frac{1}{2}\sum_m^M \sum_d^{D_m} w_{:,d}^{(m)\intercal} \overline{\overline{\alpha}}_m w_{:,d}^{(m)}\right] - E_{\alpha,Z,\tau}\left[\frac{1}{2}\sum_m^M \sum_d^{D_m} \sum_i^N \tau_m (x_{i,d}^{(m)} - w_{:,d}^{(m)\intercal} z_i)^2\right] + C_2$$

$$= -\frac{1}{2}\sum_m^M \sum_d^{D_m} w_{:,d}^{(m)\intercal} \langle \overline{\overline{\alpha}}_m \rangle w_{:,d}^{(m)} - \frac{1}{2}\sum_m^M \sum_d^{D_m} \sum_i^N \langle \tau_m \rangle (-2x_{i,d}^{(m)} w_{:,d}^{(m)\intercal} \langle z_i \rangle + w_{:,d}^{(m)\intercal} \langle z_i z_i^\intercal \rangle w_{:,d}^{(m)}) + C_3$$

$$= \sum_m^M \sum_d^{D_m} \langle \tau_m \rangle \sum_i^N w_{:,d}^{(m)\intercal} x_{i,d}^{(m)} \langle z_i \rangle - \frac{1}{2}\sum_m^M \sum_d^{D_m} w_{:,d}^{(m)\intercal} (\langle \tau_m \rangle \sum_i^N \langle z_i z_i^\intercal \rangle + \langle \overline{\overline{\alpha}}_m \rangle) w_{:,d}^{(m)} + C_3$$

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:

$$\Sigma_m^{(w)} = \left(\langle \tau_m \rangle \sum_i^N \langle z_i z_i^\intercal \rangle + \langle \overline{\overline{\alpha}}_m \rangle\right)^{-1}$$

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

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

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

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

$$= E_{W,Z}\left[\sum_m^M (a^\tau - 1)log(\tau_m) - b^\tau\tau_m\right] + E_{W,Z}\left[-\frac{1}{2}\sum_m^M\sum_i^N log(|\tau_m^{-1}\mathbf{I}|) - (x_i^{(m)} - W^{(m)\intercal}z_i)^2\tau_m\right] + C_2$$

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:

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

$$b_m^\tau = b^\tau + \sum_i^N \left\langle (x_i^{(m)} - W^{(m)\intercal}z_i)^2 \right\rangle$$

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:

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

$$= \int_{UV} log(p(U, V)) + \sum_m^M\sum_k^K\sum_d^{D_m} log\Big(\mathcal{N}(w_{k,d}^{(m)}|0, \alpha_{m,k}^{-1})\Big)dUdV$$

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

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

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

$$V' = \left[V \middle| \mathbf{1} \middle| \mu_v \right]$$

Such that $log(\alpha) = U'V'^{\intercal}$ then $\alpha_{m,k} = e^{u'_m v'^{\intercal}_k}$ 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 $\langle W^{(m)}W^{(m)\intercal}\rangle$ and thus:

$$\propto \int_{UV} 2log(p(U,V)) + \sum_{m}^{M}\sum_{k}^{K} \left(D_m u'_m v'^{\intercal}_k - \langle W^{(m)}W^{(m)\intercal}\rangle_{k,k} e^{u'_m v'^{\intercal}_k} \right) dUdV$$

The expression $L = 2log(p(U,V)) + \sum_{m}^{M}\sum_{k}^{K} \left(D_m u'_m v'^{\intercal}_k - \langle W^{(m)}W^{(m)\intercal}\rangle_{k,k} e^{u'_m v'^{\intercal}_k} \right)$ can be maximized by gradient descent provided we compute the derivatives $\frac{\delta L}{\delta U}, \frac{\delta L}{\delta \mu_u}, \frac{\delta L}{\delta V}$ and $\frac{\delta L}{\delta \mu_v}$.

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:

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

And thus we can write:

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

$$= -\lambda(tr(U^TU) + tr(V^TV)) + C$$

Such that:

$$L = \sum_{m}^{M}\sum_{k}^{K}\left(D_m u'_m v_k'^{\intercal} - \langle W^{(m)} W^{(m)\intercal}\rangle_{k,k} e^{u'_m v_k'^{\intercal}}\right) - \lambda(tr(U^T U) + tr(V^T V)) + C$$

and therefore:

$$\frac{\delta L}{\delta U} = AV + \lambda U \qquad \frac{\delta L}{\delta \mu_u} = A\mathbf{1}$$

$$\frac{\delta L}{\delta V} = A^{\intercal} U + \lambda V \qquad \frac{\delta L}{\delta \mu_v} = A^{\intercal}\mathbf{1}$$

Where:

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

$$A = D\mathbf{1}^{\intercal} - \mathbf{1}tr(\langle W^{(m)} W^{(m)\intercal}\rangle)^{\intercal} \circ exp(U'V'^{\intercal})$$

Where $\circ$ stands for the Hadamard product (element-wise matrix multiplication) and the unit vectors $\mathbf{1}$ are $K \times 1$ and $M \times 1$ respectively.

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 λ 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:

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

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:

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

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

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

Initialize $q(W), q(Z), q(\tau), U$ and V.
while not converged **do**
    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**
        $q(\alpha) \leftarrow \prod_{m=1}^M \prod_{k=1}^K \mathcal{G}(a_{m,k}^{\alpha}, b_{m,k}^{\alpha})$
    else
        $U, V \leftarrow argmax_{U,V} L$
        $\langle \alpha \rangle \leftarrow exp(U'V'^{\intercal})$
    $q(\tau) \leftarrow \prod_m^M \mathcal{G}(\tau_m | a_m^{\tau}, b_m^{\tau})$

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 refering 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 $q(W^{(m)})q(Z^*)$.