Advanced Machine Learning, Final Project

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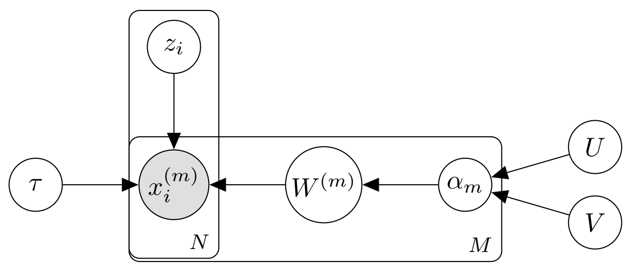
We begin by presenting the graphical model corresponding to group factor analysis:



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:

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

Where 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:

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

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:

$$= \sum_m^M (a^\tau + \frac{ND_m}{2} - 1)log(\tau_m) - \Big(b^\tau + \sum_i^N \Big\langle (x_i^{(m)} - W^{(m)\intercal} z_i)^2 \Big\rangle\Big)\tau_m + C_2$$

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:

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

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

Finally we turn our attention to U and V at which point we 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:

$$U = \Big[U \Big| \mu_u \Big| \mathbf{1}\Big]$$

$$V^\intercal = \Big[V^\intercal \Big| \mathbf{1} \Big| \mu_v\Big]$$

Such that $log(\alpha) = UV^\intercal$, so let us use the expanded version of U and V for what follows and then recall:

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

$$= \int_\Theta q(Z, W, \tau) q(U) q(V) log(\frac{p(Z, \tau, X) p(U, V) p(W|\alpha)}{q(Z, W, \tau) q(U) q(V)}) dZ dW d\tau dU dV$$

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

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

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:

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

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

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

We then express $p(W|\alpha)$ in terms of U and V as opposed to α such that $\alpha_{m,k} = e^{u_m v_k^\intercal}$ 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:

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

The expression $L = 2log(p(U,V)) + \sum_m^M \sum_k^K \left(D_m u_m v_k^\intercal - \langle W^{(m)}W^{(m)\intercal}\rangle_{k,k} e^{u_m v_k^\intercal}\right)$ can be maximized by gradient descent provided we compute the derivatives $\frac{\delta L}{\delta U}$ and $\frac{\delta L}{\delta V}$.

. . .

Recalling that $\alpha_{m,k} = e^{u_m v_k^\intercal}$ and that $log(p(U,V)) = -2\lambda(tr(U^\intercal U) + tr(V^\intercal V))$ allows us to write the expression for L above as:

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

Then if we assume λ to be negibly small 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:

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

Then in comparison 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:

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

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

And so we notice the resemblance between the solutions provided by numerical optimization and full variational inference.