S1 Appendix: Observation models for Gaussian, Poisson and multinomial

This is a supplementary material for observation models in the main manuscript, providing priors, the expectation of log-likelihood and the updating equations.

Gaussian distribution

We denote univariate Gaussian density function as $Gauss(\cdot|\mu, \sigma^2)$ where μ and σ^2 are mean and variances. We assume conjugate priors for μ and σ^2 in each cluster block:

$$s_{v,g,k} \sim \operatorname{Ga}(\cdot|\gamma_0/2,\gamma_0\sigma_0^2/2)$$

$$\mu_{v,g,k} \sim \operatorname{Gauss}(\cdot|\mu_0,(\lambda_0s_{v,g,k})^{-1}),$$

where $\operatorname{Ga}(\cdot|a, b)$ denotes Gamma distribution with shape and rate parameters (a, b). In the present paper, we set $\sigma_0^2 = 10^4$, $\gamma_0 = 1$, and $\lambda_0 = 10^{-4}$ so that the prior distributions are nearly non-informative. It can be shown that the variational approximation for the posterior $q_{\boldsymbol{\theta}^{(m)}}(\boldsymbol{\theta}^{(m)})$ is given by

$$\prod_{v=1}^{V} \prod_{g=1}^{G} \prod_{k=1}^{K} \operatorname{Gauss}(\mu_{v,g,k} | \mu_{0,v,g,k}, (\lambda_{0,v,g,k} s_{0,v,g,k})^{-1}) \times \operatorname{Ga}(s_{0,v,g,k} | \gamma_{0,v,g,k} / 2, \gamma_{0,v,g,k} \sigma_{0,v,g,k}^{2} / 2),$$

where the hyperparameters are updated by

$$\begin{split} \lambda_{0,v,g,k} &= \lambda_0 + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k} \\ \mu_{0,v,g,k} &= \frac{1}{\lambda_{0,v,g,k}} \Big\{ \lambda_0 \mu_0 + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k} X_{i,j}^{(m)} \Big\} \\ \gamma_{0,v,g,k} &= \gamma_0 + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k} \\ \sigma_{0,v,g,k}^2 &= \frac{1}{\gamma_{0,v,g,k}} \Big\{ \gamma_0 \sigma_0^2 + \lambda_0 \mu_0^2 \\ &+ \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k} (X_{i,j}^{(m)})^2 - \lambda_{0,v,g,k} \mu_{0,v,g,k}^2 \Big\}. \end{split}$$

Finally, the expectation of the conditional log-likelihood $\mathbb{E}_{q(\theta)}\left[\log p(X_{i,j}^{(m)}|\boldsymbol{\theta}_{v,g,k}^{(m)})\right]$ is given by

$$-\frac{1}{2} \bigg\{ \frac{(X_{i,j}^{(m)} - \mu_{0,v,g,k})^2}{\sigma_{0,v,g,k}^2} + \frac{1}{\lambda_{0,v,g,k}} + \log \sigma_{0,v,g,k}^2 \\ + \log(\gamma_{0,v,g,k}/2) - \psi(\gamma_{0,v,g,k}/2) + \log(2\pi) \bigg\}.$$

Poisson distribution

We denote Poisson distribution as $Poisson(\cdot|\lambda)$ where λ is a rate parameter. The conjugate prior for λ is given by

$$\lambda_{v,g,k} \sim \operatorname{Ga}(\cdot | \alpha_0, \beta_0),$$

where we set α_0 and β_0 to one. It can be shown that the variational approximation is given by

$$q_{\boldsymbol{\theta}^{(m)}}(\boldsymbol{\theta}^{(m)}) = \prod_{v=1}^{V} \prod_{g=1}^{G} \prod_{k=1}^{K} \operatorname{Ga}(\lambda_{v,g,k} | \alpha_{0,v,g,k}, \beta_{0,v,g,k}),$$

where the hyperparameters are updated by

$$\alpha_{0,v,g,k} = \alpha_0 + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k} X_{i,j}^{(m)}$$

$$\beta_{0,v,g,k} = \beta_0 + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^n \tau_{j,v,g}^{(m)} \eta_{i,v,k}.$$

The expectation of the conditional log-likelihood becomes

$$X_{i,j}^{(m)} \{ \psi(\alpha_{0,v,g,k}) - \psi(\beta_{0,v,g,k}) \} - \frac{\alpha_{0,v,g,k}}{\beta_{0,v,g,k}} - \sum_{t=1}^{X_{i,j}^{(m)}} \log t.$$

Categorical/multinomial distribution

For a categorical feature x ($x \in \{c_1, \ldots, c_H\}$), we denote categorical distribution as $\operatorname{Cat}(\cdot | \boldsymbol{p})$ where H is the number of categories, and $\boldsymbol{p} = (p_1, \ldots, p_H)$ are probabilities for each category with $\sum_{h=1}^{H} p_h = 1$. We assume the conjugate prior for (p_1, \ldots, p_H) ,

$$(p_1,\ldots,p_H) \sim \text{Dirichlet}(\cdot|\boldsymbol{\rho}_0),$$

where $\text{Dirichlet}(\cdot|\boldsymbol{\rho}_0)$ denotes a Dirichlet distribution with prior sample size $\boldsymbol{\rho}_0$. We set $\boldsymbol{\rho}_0$ to $(1, \ldots, 1)$. It can be shown that

$$q_{\boldsymbol{\theta}^{(m)}}(\boldsymbol{\theta}^{(m)}) = \prod_{v=1}^{V} \prod_{g=1}^{G} \prod_{k=1}^{K} \text{Dirichlet}(\boldsymbol{p}_{v,g,k} | \boldsymbol{\rho}_{0,v,g,k}),$$

where the hyperparameters are updated by

$$\rho_{0,v,g,k,h} = \rho_{0,h} + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^{n} \tau_{j,v,g}^{(m)} \eta_{i,v,k} \mathbb{I}(X_{i,j}^{(m)} = c_h),$$

where $\rho_{0,v,g,k,h}$ denotes the *h*th element of $\rho_{0,v,g,k}$. The expectation of the log-likelihood is then given by

$$\sum_{h=1}^{H} \mathbb{I}(X_{i,j}^{(m)} = c_h) \{ \psi(\rho_{0,h,v,g,k}) - \psi(\sum_{h'=1}^{H} \rho_{0,h',v,g,k}) \}.$$

Since the categorical distribution differs depending on the number of categories H, we need to define different types of categorical distribution. Alternatively, for the purpose of simplicity, we can set H to the maximum number of categories for different categorical features, and fit a single family of categorical distribution to all these features.

More generally, in the case of multinomial distribution, the update equation and the expectation of the log-likelihood becomes

$$\rho_{0,v,g,k,h} = \rho_{0,h} + \sum_{j=1}^{d^{(m)}} \sum_{i=1}^{n} \tau^{(m)} \eta_{i,v,k} n_{i,j,h}$$

$$\sum_{h=1}^{H} n_{i,j,h} \{ \psi(\rho_{0,h,v,g,k}) - \psi(\sum_{h'=1}^{H} \rho_{0,h',v,g,k}) \}$$

$$+ \log \left(\sum_{n_{i,j,1},\dots,n_{i,j,H}}^{H} \right),$$

where $n_{i,j,h}$ is the number of category c_h in $X_{i,j}^{(m)}$; the last term is the logarithm of multinomial coefficients.