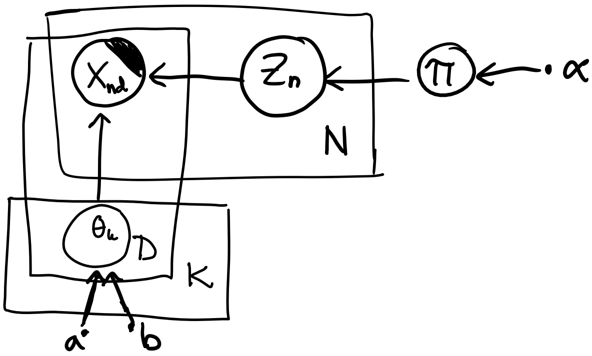
Bernoulli Mixture Model

den 8 november 2023 14:14

a)



Let $\theta_k = (\theta_1, \dots, \theta_d)$

b) $\log p(X, Z, \pi, \theta)$

Start with conditioning on X:

$$\log p(X,Z,\pi,\theta) = \log p(X|Z,\pi,\theta)\, p(Z,\pi,\theta)$$

$$= \log p(X|Z,\theta) + \log p(Z|\pi) + \log p(\pi) + \log p(\theta)$$

$$p(X|Z,\theta) = \prod_{n=1}^{N} \prod_{k=1}^{K} p(X_n = x_n | Z_n = k, \theta_k)^{\mathbb{1}\{Z_n = k\}} = \prod_{n=1,\, k=1}^{N,K} \left(\prod_{d=1}^{D} p(X_{nd} = x_{nd} | Z_n = k, \theta_{kd}) \right)^{\mathbb{1}\{Z_n = k\}}$$

$$= \prod_{n,k}^{N,K} \left(\prod_{d=1}^{D} \left(\theta_{kd}^{x_{nd}} (1-\theta_{kd})^{1-x_{nd}} \right) \right)^{\mathbb{1}\{Z_n = k\}}$$

$$\Rightarrow \log p(X|Z,\theta) = \sum_{n,k}^{N,K} z_n^k \left(\sum_{d=1}^{D} x_{nd} \log \theta_{kd} + (1-x_{nd}) \log(1-\theta_{kd}) \right)$$

↳ shorter notation for $\mathbb{1}\{Z_n = k\}$

$$= \sum_{n,k}^{N,K} z_n^k \left(\sum_{d=1}^{D} x_{nd} \log \theta_{kd} + \sum_{d=1}^{D} (1 - x_{nd}) \log(1-\theta_{kd}) \right)$$

$$\log p(Z|\pi) = \sum_{n=1,\, k=1}^{N,K} z_n^k \log \pi_k$$

$$\log p(\pi) = \log \left(\frac{1}{B(\alpha)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1} \right) = -\cancel{\log B(\alpha)} + \sum_{k=1}^{K} (\alpha_k - 1) \log \pi_k$$

$\pm$

$$\log p(\theta) = \log \prod_{k,d}^{K,D} p(\theta_{kd}) \stackrel{\pm}{=} \sum_{k=1}^{K} \sum_{d=1}^{D} (a_k - 1) \log \theta_{kd} - (b_k - 1) \log 1 - \theta_{kd} - \log \cancel{B(a_k, b_k)}$$

$\pm$

c) Mean-field approximation: $q(Z,\pi,\theta) = q(Z)\, q(\pi)\, q(\theta)$ (*)

Generally, we want to do as few assumptions as possible while still being able to solve the CAVI update equations.

That is why we avoid e.g. $q(Z,\pi,\theta) = \prod_{n=1}^{N} q(z_n)\, q(\pi) \prod_{k=1}^{K} q(\theta_k)$

However, $q(Z,\pi,\theta) = q(Z)\, q(\pi,\theta)$ would have been sufficient. For this exercise (*) is more clear.

d) Lets derive the CAVI updates for $q(Z)$, $q(\pi)$ and $q(\theta)$

$$\log q(\theta)^* = \mathbb{E}_{-\theta}[\log p(X,Z,\theta,\pi)] = \mathbb{E}_{-\theta}[\log p(X|Z,\theta) + \log p(\theta) + \cancel{\log p(Z|\pi)} + \cancel{\log p(\pi)}]$$

$$\stackrel{+}{=} \mathbb{E}_{-\theta}[\log p(X|Z,\theta) + \log p(\theta)] = \mathbb{E}_{-\theta}[\log p(X|Z,\theta)] + \mathbb{E}_{-\theta}[\log p(\theta)]$$

$$= \underbrace{\mathbb{E}_{-\theta}[\log p(X|Z,\theta)]}_{1} + \underbrace{\log p(\theta)}_{2}$$

$$= \mathbb{E}_{Z,\pi}\left[\sum_{n=1}^{N}\sum_{k=1}^{K} z_n^k \left(x_n^D \log \theta_k + (D - x_n^D) \log 1-\theta_k\right)\right]$$

$$= \sum_{n,k}^{N,K} \underbrace{\mathbb{E}_Z[z_n^k]} (x_n^D \log \theta_k + (D - x_n^D) \log(1-\theta_k))$$

$\mathbb{E}[\mathbb{1}(A=a)]$

$= \mathbb{P}(A=a) \rightarrow \mathbb{E}_Z[\mathbb{1}\{z_n=k\}]$

$= q(z_n = k)$

$$\Rightarrow 1 + 2 = \sum_{n,k}^{N,K} q(z_n=k)\left[\sum_{d=1}^{D} x_{nd} \log \theta_{kd} + (1-x_{nd}) \log(1-\theta_{kd})\right] + \sum_{k=1}^{K}\sum_{d=1}^{D} (a-1)\log\theta_{kd} + (b-1)\log 1-\theta_{kd}$$

$$= \left\{\begin{array}{l}\text{We suspect } q^*(\theta) \\ \text{in same form as} \\ \text{prior, so we rewrite} \\ \text{on same form as } 2\end{array}\right\} = \sum_{k=1}^{K}\left\{\sum_{n=1}^{N} q(z_n=k)\sum_{d=1}^{D} x_{nd} \log \theta_k + \sum_{d=1}^{D}(a-1)\log\theta_{kd}\right.$$

$$+ \sum_{n=1}^{N} q(z_n=k) \underbrace{\sum_{d=1}^{D} (1-x_{nd}) \log(1-\theta_{kd})} + \underbrace{\sum_{d=1}^{D} (b-1) \log(1-\theta_{kd})} \Big\}$$

$$= \sum_{k=1}^{K} \sum_{d=1}^{D} \Big\{ \Big(\underbrace{\sum_{n=1}^{N} \left[q(z_n=k) x_{nd} \right] + a - 1}_{a^*_{kd}} \Big) \log \theta_{kd} + \Big(\underbrace{\sum_{n=1}^{N} \left[q(z_n=k)(1-x_{nd}) \right] + b - 1}_{b^*_{kd}} \Big) \log(1-\theta_{kd}) \Big\}$$

By comparing to $\log p(\theta)$, we see that $\log q^*(\theta)$ is on the form of $k \times d$ independent Beta-distributions with parameters a^* and b^*,

i.e. $q^*(\theta) = \prod_{k,d}^{K,D} q^*(\theta_{kd})$

where $$q^*(\theta_k) = \mathrm{Beta}\Big(\underbrace{\sum_{n=1}^{N} \left[q(z_n=k) x_{nd} \right] + a - 1}_{\equiv \hat{a}_{kd}}, \underbrace{\sum_{n=1}^{N} \left[q(z_n=k)(1-x_{nd}) \right] + b - 1}_{\tilde{b}_{kd}} \Big)$$

We will now do $q(z)$ and $q(\pi)$ in little less detail.

$$\log q^*(z) \stackrel{+}{=} \mathbb{E}_{-z}\left[\log p(X|z,\theta) + \log p(z|\pi) \right] =$$

$$= \underbrace{\mathbb{E}_{\theta}\left[\log p(X|z,\theta) \right]}_{①} + \underbrace{\mathbb{E}_{\pi}\left[\log p(z|\pi) \right]}_{②}$$

$$① = \mathbb{E}_{\theta}\left[\sum_{n=1}^{N} \sum_{k=1}^{K} z_n^k \left(\sum_{d=1}^{D} x_{nd} \log \theta_{kd} + (1-x_{nd}) \log 1-\theta_{kd} \right) \right]$$

$$= \sum_{n,k}^{N,K} z_n^k \left(\sum_{d=1}^{D} x_{nd} \mathbb{E}_{\theta}\left[\log \theta_{kd} \right] + (1-x_{nd}) \cdot \mathbb{E}_{\theta}\left[\log 1-\theta_{kd} \right] \right)$$

$$\Rightarrow ① + ② = \sum_{n,k}^{N,K} z_n^k \left(\sum_{d=1}^{D} x_{nd} \mathbb{E}_{\theta}\left[\log \theta_{kd} \right] + (1-x_{nd}) \mathbb{E}_{\theta}\left[\log 1-\theta_{kd} \right] \right) + \mathbb{E}_{\pi}\left[\sum_{n=1, k=1}^{N,K} z_n^k \log \pi_k \right]$$

only $\mathbb{E}_{\theta_{kd}}$ hits $\log \theta_{kd}$

$$= \sum_{n,k}^{N,K} z_n^k \Big(\underbrace{\sum_{d=1}^{D} x_{nd} \mathbb{E}_{\theta_{kd}}\left[\log \theta_{kd} \right] + (1-x_{nd}) \mathbb{E}_{\theta_{kd}}\left[\log 1-\theta_{kd} \right] + \mathbb{E}_{\pi}\left[\log \pi_k \right]}_{\equiv \log \rho_{nk}} \Big)$$

$$\Rightarrow q^*(z) \propto \prod_{n,k}^{N,K} \rho_{nk}^{z_{nk}} \quad \Rightarrow \quad q^*(z) = \prod_{\substack{n=1\\k=1}}^{N,K} r_{nk}^{z_{nk}}, \quad r_{nk} = \frac{\rho_{nk}}{\sum_{j=1}^{K} \rho_{nj}}$$

{ See Bishop section 10.2.1 for more details on these steps }

Also, since we've already shown $q(\theta_{kd}) = \text{Beta}(\tilde{a}_{kd}, \tilde{b}_{kd})$

digamma-function

we can evaluate $\mathbb{E}_{\theta_{kd}}\left[\log \theta_{kd}\right] = \left\{ \begin{array}{c}\text{Wikipedia}\\ \text{Beta-dist.}\end{array} \right\} = \psi(\tilde{a}_{kd}) - \psi(\tilde{a}_{kd} + \tilde{b}_{kd})$

and $\mathbb{E}_{\theta_{kd}}\left[\log (1-\theta_{kd})\right] = \psi(\tilde{b}_{kd}) - \psi(\tilde{a}_{kd} + \tilde{b}_{kd})$

$\mathbb{E}_\pi[\log \pi]$ we can only evaluate after analyzing $q(\pi)$:

$$\log q^*(\pi) \overset{+}{=} \mathbb{E}_{-\pi}\left[\log p(z|\pi) + \log p(\pi)\right] = \mathbb{E}_z\left[\log p(z|\pi)\right] + \log p(\pi)$$

$$\overset{+}{=} \sum_{n,k}^{N,K} \mathbb{E}_z[z_{nk}] \log \pi_k + \sum_{k=1}^{K} (\alpha_k - 1) \log \pi_k = \sum_{k=1}^{K} \left(\sum_{n=1}^{N} q(z_n{=}k) + \alpha_k - 1 \right) \log \pi_k$$

$$\Rightarrow q^*(\pi) = \text{Dir}\Big(\underbrace{\sum_{n=1}^{N} q(z_{nk}) + \alpha_k}_{\equiv \tilde{\alpha}} \Big)$$

$\sum_{k=1}^{K} \tilde{\alpha}_i$

Now, we can also calculate $\mathbb{E}_\pi\left[\log \pi_k\right] = \psi(\tilde{\alpha}_k) - \psi(\tilde{\alpha}_0)$

In summary:

$$q(\theta) = \prod_{\substack{k=1\\d=1}}^{K,D} q(\theta_{kd}), \quad q(\theta_{kd}) = \text{Beta}(\tilde{a}_{kd}, \tilde{b}_{kd}), \quad \left\{ \begin{array}{l} \tilde{a}_{kd} = \sum_{n=1}^{N} \left[q(z_n{=}k) x_{nd} \right] + a \\ \tilde{b}_{kd} = \sum_{n=1}^{N} \left[q(z_n{=}k)(1 - x_{nd}) \right] + b \end{array} \right.$$

$$q(z) = \prod_{n=1}^{N} q(z_n), \quad q(z_n) = \text{Cat}(r_{n1}, \dots, r_{nK}), \quad r_{nk} = \frac{\rho_{nk}}{\sum_{j=1}^{K} \rho_{nj}}$$

$$\log \rho_{nk} = \sum_{d=1}^{D} x_{nd}\left(\psi(\tilde{a}_{kd}) - \psi(a_{kd} + \tilde{b}_{kd})\right) + (1 - x_{nd})\left(\psi(\tilde{b}_{kd}) - \psi(\tilde{b}_{kd} + \tilde{a}_{kd})\right) + \psi(\tilde{\alpha}_{k}) - \psi(\tilde{\alpha}_0)$$

$$q(\pi) = \text{Dir}(\tilde{\alpha}), \quad \tilde{\alpha} = \sum_{n=1}^{N} \underbrace{q(z_n{=}k)}_{= r_{nk}} + \alpha_k$$

ELBO

$$\mathcal{L} = \mathbb{E}_{q(z)q(\theta)q(\pi)}\left[\log \frac{p(X,z,\theta,\pi)}{q(z,\theta,\pi)}\right] = \mathbb{E}_{q(z)q(\theta)q(\pi)}\left[\log p(X|z,\theta)\right] \quad ①$$

$$+ \mathbb{E}_{q(z)q(\pi)}\left[\log p(z|\pi)\right] \; ② + \mathbb{E}_{q(\pi)}\left[\log p(\pi)\right] \; ③ + \mathbb{E}_{q(\theta)}\left[\log p(\theta)\right] \; ④$$

$$- \mathbb{E}_{q(z)}\left[\log q(z)\right] \; ⑤ - \mathbb{E}_{q(\pi)}\left[\log q(\pi)\right] \; ⑥ - \mathbb{E}_{q(\theta)}\left[\log q(\theta)\right] \; ⑦$$

← recall the expressions we derived in b)

$$① = \mathbb{E}_{q(z)q(\theta)}\left[\log \prod_{n,k}^{N,K}\left(\prod_{d=1}^{D}\left(\theta_{k}^{x_{nd}}(1-\theta_k)^{1-x_{nd}}\right)\right)^{1\{z_n=k\}}\right] =$$

$$= \sum_{n,k} \mathbb{E}_{q(z)q(\theta)}\left[1\{z_n=k\}\left(\sum_d x_{nd}\log\theta_{kd} + (1-x_{nd})\log 1-\theta_{kd}\right)\right] =$$

$$= \sum_{n,k} q(z_n=k)\left(\sum_d x_{nd}\mathbb{E}_\theta\left[\log\theta_{kd}\right] + (1-x_{nd})\mathbb{E}_\theta\left[\log 1-\theta_{kd}\right]\right)$$

$$② = \mathbb{E}_{q(z)q(\pi)}\left[\sum_{n=1,k=1}^{N,K} z_n^k \log \pi_k\right] = \sum_{n=1,k=1}^{N,K} q(z_n=k)\,\mathbb{E}_\pi\left[\log\pi_k\right]$$

$$③ = \mathbb{E}_{q(\pi)}\left[-\log B(\alpha) + \sum_{k=1}^{K}(\alpha_k-1)\log\pi_k\right] = -\log B(\alpha) + \sum_{k=1}^{K}(\alpha_k-1)\mathbb{E}_\pi\left[\log\pi_k\right]$$

$$④ = \mathbb{E}_{q(\theta)}\left[\sum_{k=1}^{K}(a_k-1)\log\theta_k + (b_k-1)\log 1-\theta_k - B(a_k,b_k)\right] = \sum_{k=1}^{K}(a_k-1)\mathbb{E}_\theta\left[\log\theta_k\right] + (b_k-1)\mathbb{E}_\theta\left[\log 1-\theta_k\right]$$
$$- \log B(a_k,b_k)$$

⑤, ⑥, ⑦ are entropies and we can look them up on Wikipedia (except ⑤)

$$⑤ = \mathbb{E}_{q(z)}\left[\sum_{n=1,k=1}^{N,K}\log r_{nk}^{1\{z_n=k\}}\right] = \sum_{n,k}^{N,K} q(z_n=k)\log q(z_n=k)$$

entropy

$$⑥ = H_{q(\pi)}[\pi] = \{\text{Wikipedia}\} = \log B(\tilde{\alpha}) + (\tilde{\alpha}_0 - K)\psi(\tilde{\alpha}_0) - \sum_{j=1}^{K}(\tilde{\alpha}_j-1)\psi(\tilde{\alpha}_j)$$

$$⑦ = H_{q(\theta)}[\theta] = \sum_{k=1}^{K} H_{q(\theta_k)}[\theta_k] = \{\text{wikipedia}\} = \sum_{k=1}^{K}\log B(\tilde{a}_k,\tilde{b}_k) - (\tilde{a}_k-1)\psi(\tilde{a}_k) - (\tilde{b}_k-1)\psi(\tilde{b}_k)$$
$$+ (\tilde{a}_k+\tilde{b}_k-2)\psi(\tilde{a}_k+\tilde{b}_k)$$