

# LATENT DISCRETE GRAPHICAL MODEL

Measurement  $M$ , latent state  $L$ , parameters  $\Theta = (\delta, \gamma, \theta, \rho, D)$ , case/control indicator  $Y$ .

$$\text{Bronze standard only } [M, L, \Theta] = \{\prod_{k=1}^K [M_k | L_k, \Theta]\} [L | \Theta] [\Theta]$$

$$[M, L, \Theta] \propto \exp \left\{ \sum_{k=1}^K \left[ \log(1 - \delta_k) + M_k \log \frac{\delta_k}{1 - \delta_k} + Y L_k \log \frac{1 - \gamma_k}{1 - \delta_k} + Y L_k M_k \log \frac{\gamma_k (1 - \delta_k)}{\delta_k (1 - \gamma_k)} \right] + Y \left[ \sum_{k=1}^K (L_k \theta_k + \rho \sum_{k' \neq k} L_k L_{k'} D_{kk'}) - A(\theta, \rho, D) \right] \right\} [\Theta]$$

Variational approximate posterior distribution of  $\Theta$ .

Assume the approximate posterior  $Q(\Theta, L)$  to be fully factorized, i.e.

$$Q(\Theta, L) = q(\delta, \gamma) q(L) q(\theta) q(\rho) q(D) = \prod_{\eta \in \{\Theta, L\}} q(\eta)$$

We maximize the lower bound of the joint density (minimize the KL divergence) to find  $Q$ .

$$Q(\Theta, L) = \operatorname{argmax}\{\mathbb{E}_Q \left[ \log \frac{[M, L, \Theta]}{Q(\Theta, L)} \right]\}$$

$$q(\eta) \propto \exp\{\mathbb{E}_{Q(-\eta)} (\log[M, L, \Theta])\}$$

For  $q(\gamma, \delta)$ :

$$\begin{aligned}
q(\delta, \gamma) &\propto \exp \left\{ \mathbb{E}_L \left[ \sum_{k=1}^K \log[M_k | L_k, \delta, \gamma] + \log[\delta, \gamma] \right] \right\} \\
&\propto \exp \left\{ \sum_{k=1}^K \left[ \log(1 - \delta_k) + M_k \log \frac{\delta_k}{1 - \delta_k} + Y q_{l_k} \left( \log \frac{1 - \gamma_k}{1 - \delta_k} \right) + Y q_{l_k} M_k \log \frac{\gamma_k (1 - \delta_k)}{\delta_k (1 - \gamma_k)} \right] \right\} [\gamma, \delta] \\
&= \prod_{k=1}^K \left[ (1 - \gamma_k)^{Y q_{l_k} (1 - M_k)} \gamma_k^{Y q_{l_k} M_k} \right] \left[ (1 - \delta_k)^{1 + Y q_{l_k} M_k - Y q_{l_k} - M_k} \delta_k^{M_k (1 - Y q_{l_k})} \right] [\gamma, \delta]
\end{aligned}$$

Where  $q_{l_k} = \mathbb{E}_Q(L_k)$ . Let  $a_k^*, b_k^*$  be the hyper-parameters for  $\gamma_k$ , and let  $c_k^*, d_k^*$  be the hyper-parameters for  $\delta_k$ . Then the posterior distribution is:  $\gamma_k \sim \text{Beta}(A_k^*, B_k^*)$  and  $\delta_k \sim \text{Beta}(A'_k, B'_k)$  where

$$\begin{aligned}
A_k^* &= Y q_{l_k} M_k + a_k^* \\
B_k^* &= Y q_{l_k} (1 - M_k) + b_k^* \\
A'_K &= M_k (1 - Y q_{l_k}) + c_K^* \\
B'_K &= 1 + Y q_{l_k} M_k - Y q_{l_k} - M_k + d_K^*
\end{aligned}$$

With  $n$  independent samples:

$$\begin{aligned}
A_{kn}^* &= \sum_{i=1}^n Y_i q_{l_{ik}} M_{ik} + a_k^* \\
B_{kn}^* &= \sum_{i=1}^n Y_i q_{l_{ik}} (1 - M_{ik}) + b_k^* \\
A'_{kn} &= \sum_{i=1}^n M_{ik} (1 - Y_i q_{l_{ik}}) + c_K^* \\
B'_{kn} &= n + \sum_{i=1}^n (Y_i q_{l_{ik}} M_{ik} - Y_i q_{l_{ik}} - M_{ik}) + d_K^*
\end{aligned}$$

For  $q(L)$ :

$$\begin{aligned}
q(L) &= \prod_k q(L_k) \propto \exp \left\{ \mathbb{E}_{\Theta} \left[ \sum_{k=1}^K \log[M_k | L_k, \delta, \gamma] + \log[L | \theta, \rho, D] \right] \right\} \\
&= \exp \left\{ Y \mathbb{E} \sum_{k=1}^K \left[ L_k (\theta_k + \log \frac{1-\gamma_k}{1-\delta_k} + M_k \log \frac{\gamma_k(1-\delta_k)}{\delta_k(1-\gamma_k)}) + \rho \sum_{k' \neq k} L_k L_{k'} D_{kk'} \right] \right\}
\end{aligned}$$

Let  $h_k = \theta_k + \log \frac{1-\gamma_k}{1-\delta_k} + M_k \log \frac{\gamma_k(1-\delta_k)}{\delta_k(1-\gamma_k)}$ , and let  $d_{kk'} = \mathbb{E}_Q(D_{kk'})$ , then

$$\begin{aligned}
q(L_k) &\propto \exp \left\{ Y \left[ L_k \mathbb{E}(h_k) + \rho L_k \sum_{k' \neq k} q_{l_{k'}} d_{kk'} \right] \right\} \\
q_{l_k} &= \frac{\exp[Y(H_k + \mu_\rho \sum_{k' \neq k} q_{l_{k'}} d_{kk'})]}{1 + \exp[Y(H_k + \mu_\rho \sum_{k' \neq k} q_{l_{k'}} d_{kk'})]}
\end{aligned}$$

Where with  $\psi(x) = \frac{\partial \log \Gamma(x)}{\partial x}$  and  $\psi(x+y) = \frac{\partial \log \Gamma(x+y)}{\partial x}$

$$\begin{aligned}
H_k &= \mathbb{E}_Q(h_k) = M_k [\psi(A_k^*) - \psi(A'_k)] + (1 - M_k) [\psi(B_k^*) - \psi(B'_k)] \\
&\quad + \mu_{\theta_k} - \psi(A_k^* + B_k^*) + \psi(A'_k + B'_k)
\end{aligned}$$

with  $n$  independent samples, indexed by  $i$ :

$$\begin{aligned}
q_{l_{ik}} &= \frac{\exp[Y_i(H_{ik} + \mu_\rho \sum_{k' \neq k} q_{l_{ik'}} d_{kk'})]}{1 + \exp[Y_i(H_{ik} + \mu_\rho \sum_{k' \neq k} q_{l_{ik'}} d_{kk'})]} \\
H_{ik} &= M_{ik} [\psi(A_{kn}^*) - \psi(A'_{kn})] + (1 - M_{ik}) [\psi(B_{kn}^*) - \psi(B'_{kn})] \\
&\quad + \mu_{\theta_k} - \psi(A_{kn}^* + B_{kn}^*) + \psi(A'_{kn} + B'_{kn})
\end{aligned}$$

For  $q(\theta)$ :

$$\begin{aligned}
q(\theta) &= \prod_k q(\theta_k) \propto \exp \left\{ Y \mathbb{E}_{(L, \rho, D)} \left[ \sum_{k=1}^K L_k \theta_k - A(\theta, \rho, D) \right] \right\} [\theta] \\
&\approx \exp \left\{ Y \sum_{k=1}^K \left[ q_{l_k} \theta_k - \mathbb{E} \log \left( 1 + \exp(\theta_k + \rho \sum_{k' \neq k} L_{k'} D_{kk'}) \right) \right] \right\} [\theta] \text{ by pseudo-likelihood}
\end{aligned}$$

By taylor expansion,

$$\mathbb{E}_y \log(1 + e^{x+y}) = \log(1 + e^{x+\mu_y}) + \frac{e^{x+\mu_y}}{2(1 + e^{x+\mu_y})^2} \text{Var}(y) + \mathbb{E}_y [o(y - \mu_y)^3]$$

Let  $R_k = \sum_{k' \neq k} L_{k'} D_{kk'}$ , then

$$\begin{aligned}
\mathbb{E}(R_k) &= \sum_{k' \neq k} q_{l_{k'}} d_{kk'} \\
\text{Var}(R_k) &= \sum_{k' \neq k} q_{l_{k'}} d_{kk'} (1 - q_{l_{k'}} d_{kk'}) \\
\text{Var}(\rho R_k) &= \mathbb{E}(\rho^2) \mathbb{E}(R_k^2) - \mathbb{E}(\rho)^2 \mathbb{E}(R_k)^2 \\
&= (\sigma_\rho^2 + \mu_\rho^2) [\text{Var}(R_k) + \mathbb{E}(R_k)^2] - \mu_\rho^2 \mathbb{E}(R_k)^2 \\
&= (\sigma_\rho^2 + \mu_\rho^2) \sum_{k' \neq k} q_{l_{k'}} d_{kk'} (1 - q_{l_{k'}} d_{kk'}) + \sigma_\rho^2 \left[ \sum_{k' \neq k} q_{l_{k'}} d_{kk'} \right]^2
\end{aligned}$$

Thus,  $q(\theta_k)$  is further approximated by

$$q(\theta_k) \propto \exp \left\{ Y \left[ q_{l_k} \theta_k - \log(1 + e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{k'}} d_{kk'}}) - \frac{e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{k'}} d_{kk'}}}{2(1 + e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{k'}} d_{kk'}})^2} \text{Var}(\rho R_k) \right] - \frac{1}{2} (\theta_k - \mu_\theta^*)^2 \tau_\theta^* \right\}$$

with  $n$  independent samples:

$$\begin{aligned}
q(\theta_k) &\propto \exp \left\{ \sum_{i=1}^n Y_i \left[ q_{l_{ik}} \theta_k - \log(1 + e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{ik'}} d_{kk'}}) - \frac{e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{ik'}} d_{kk'}}}{2(1 + e^{\theta_k + \mu_\rho \sum_{k' \neq k} q_{l_{ik'}} d_{kk'}})^2} \text{Var}(\rho R_{ik}) \right] - \frac{1}{2} (\theta_k - \mu_\theta^*)^2 \tau_\theta^* \right\} \\
\text{Var}(\rho R_{ik}) &= (\sigma_\rho^2 + \mu_\rho^2) \sum_{k' \neq k} q_{l_{ik'}} d_{kk'} (1 - q_{l_{ik'}} d_{kk'}) + \sigma_\rho^2 \left[ \sum_{k' \neq k} q_{l_{ik'}} d_{kk'} \right]^2
\end{aligned}$$

Then  $\mu_{\theta_k} \approx \operatorname{argmax} q(\theta_k)$ , and  $\sigma_{\theta_k}^2 \approx -\left[\frac{\partial^2 \log q(\theta_k)}{\partial \theta_k^2}\Big|_{\theta_k=\mu_{\theta_k}}\right]^{-1}$ .

For  $q(\rho)$ :

$$\begin{aligned} q(\rho) &\propto \exp \left\{ Y \mathbb{E}_{(\theta, L, D)} \left[ \rho \sum_{k=1}^K \sum_{k' \neq k} L_k L_{k'} D_{kk'} - A(\theta, \rho, D) \right] \right\} [\rho] \\ &\approx \exp \left\{ Y \rho \sum_{k=1}^K \left[ \sum_{k' \neq k} q_{l_k} q_{l_{k'}} d_{kk'} - \mathbb{E} \log \left( 1 + \exp(\theta_k + \rho \sum_{k' \neq k} L_{k'} D_{kk'}) \right) \right] \right\} [\rho] \end{aligned}$$

By Le Cam's theorem,  $R_k$  can be approximated by Poisson( $\sum_{k' \neq k} q_{l_{k'}} d_{kk'}$ ), thus

$$q(\rho) \propto \exp \left\{ Y \rho \sum_{k=1}^K \left[ \sum_{k' \neq k} q_{l_k} q_{l_{k'}} d_{kk'} - \sum_{j=0}^{K-1} \text{Poi}(j; \lambda = \sum_{k' \neq k} q_{l_{k'}} d_{kk'}) \left( \log(1 + e^{\mu_{\theta_k} + j\rho}) + \frac{e^{\mu_{\theta_k} + j\rho}}{2(1 + e^{\mu_{\theta_k} + j\rho})^2} \sigma_{\theta_k}^2 \right) \right] \right\} [\rho]$$

With  $n$  independent samples:

$$q(\rho) \propto \exp \left\{ \rho \sum_{i=1}^n Y_i \sum_{k=1}^K \left[ \sum_{k' \neq k} q_{l_{ik}} q_{l_{ik'}} d_{kk'} - \sum_{j=0}^{K-1} \text{Poi}(j; \lambda = \sum_{k' \neq k} q_{l_{ik'}} d_{kk'}) \left( \log(1 + e^{\mu_{\theta_k} + j\rho}) + \frac{e^{\mu_{\theta_k} + j\rho}}{2(1 + e^{\mu_{\theta_k} + j\rho})^2} \sigma_{\theta_k}^2 \right) \right] \right\} [\rho]$$

Then  $\mu_\rho \approx \operatorname{argmax} q(\rho)$ , and  $\sigma_\rho^2 \approx -\left[\frac{\partial^2 \log q(\rho)}{\partial \rho^2}\Big|_{\rho=\mu_\rho}\right]^{-1}$ .

For  $q(D)$ :

$$\begin{aligned} q(D) &\propto \exp \left\{ Y \mathbb{E}_{(\theta, L, \rho)} \left[ \rho \sum_{k=1}^K \sum_{k' \neq k} L_k L_{k'} D_{kk'} - A(\theta, \rho, D) \right] \right\} [D] \\ &\approx \exp \left\{ Y \rho \sum_{k=1}^K \left[ \sum_{k' \neq k} q_{l_k} q_{l_{k'}} d_{kk'} - \mathbb{E} \log \left( 1 + \exp(\theta_k + \rho \sum_{k' \neq k} L_{k'} D_{kk'}) \right) \right] \right\} [D] \\ q(D_{k_1 k_2}) &\propto \exp \left\{ 2Y \mu_\rho q_{l_{k_1}} q_{l_{k_2}} D_{k_1 k_2} - Y \mathbb{E} \log \left( 1 + e^{\theta_{k_1} + \rho \sum_{k \neq k_1, k \neq k_2} L_k D_{kk_1} + \rho L_{k_2} D_{k_1 k_2}} \right) \right. \\ &\quad \left. - Y \mathbb{E} \log \left( 1 + e^{\theta_{k_2} + \rho \sum_{k \neq k_1, k \neq k_2} L_k D_{kk_2} + \rho L_{k_1} D_{k_1 k_2}} \right) + D_{k_1 k_2} \mathbb{E}_{\pi_d} \left( \log \frac{\pi_d}{1 - \pi_d} \right) \right\} \end{aligned}$$

Let  $S_{k_1 k_2} = \theta_{k_1} + \rho \sum_{k \neq k_1, k \neq k_2} L_k D_{kk_1}$ ,  $T_{k_1 k_2} = \mathbb{E} \log(1 + e^{S_{k_1 k_2} + \rho L_{k_2}})$ ,  $T'_{k_1 k_2} = \mathbb{E} \log(1 + e^{S_{k_1 k_2}})$ , and let  $A_{\pi_d}, B_{\pi_d}$  be the Beta hyper-parameters for  $\pi_d$ , then for all  $k_1 < k_2$ :

$$\begin{aligned}\mathbb{E}_{\pi_d}(\log \frac{\pi_d}{1 - \pi_d}) &= \psi(A_{\pi_d}) - \psi(B_{\pi_d}) \\ \text{Var}(S_{k_1 k_2}) &= \sigma_{\theta_{k_1}}^2 + (\sigma_\rho^2 + \mu_\rho^2) \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1} (1 - q_{l_k} d_{kk_1}) + \sigma_\rho^2 \left[ \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1} \right]^2 \\ \text{Var}(\rho L_k) &= (\sigma_\rho^2 + \mu_\rho^2) q_{l_k} - \mu_\rho^2 q_{l_k}^2\end{aligned}$$

Thus

$$\begin{aligned}T_{k_1 k_2} &\approx \log(1 + e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1} + \mu_\rho q_{l_{k_2}}}) + \frac{e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1} + \mu_\rho q_{l_{k_2}}}}{2(1 + e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1} + \mu_\rho q_{l_{k_2}}})^2} [\text{Var}(S_{k_1 k_2}) + \text{Var}(\rho L_{k_2})] \\ T'_{k_1 k_2} &\approx \log(1 + e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1}}) + \frac{e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1}}}{2(1 + e^{\mu_{\theta_{k_1}} + \mu_\rho \sum_{k \neq k_1, k \neq k_2} q_{l_k} d_{kk_1}})^2} \text{Var}(S_{k_1 k_2}) \\ d_{k_1 k_2} &= \frac{\exp \{ 2Y \mu_\rho q_{l_{k_1}} q_{l_{k_2}} - YT_{k_1 k_2} - YT_{k_2 k_1} + \psi(A_{\pi_d}) - \psi(B_{\pi_d}) \}}{\exp \{ 2Y \mu_\rho q_{l_{k_1}} q_{l_{k_2}} - YT_{k_1 k_2} - YT_{k_2 k_1} + \psi(A_{\pi_d}) - \psi(B_{\pi_d}) \} + \exp \{ -YT'_{k_1 k_2} - YT'_{k_2 k_1} \}}\end{aligned}$$

With  $n$  independent samples:

$$d_{k_1 k_2} = \frac{\exp \{ \sum_{i=1}^n Y_i [2\mu_\rho q_{l_{ik_1}} q_{l_{ik_2}} - T_{k_1 k_2}^{(i)} - T_{k_2 k_1}^{(i)}] + \psi(A_{\pi_d}) - \psi(B_{\pi_d}) \}}{\exp \{ \sum_{i=1}^n Y_i [2\mu_\rho q_{l_{ik_1}} q_{l_{ik_2}} - T_{k_1 k_2}^{(i)} - T_{k_2 k_1}^{(i)}] + \psi(A_{\pi_d}) - \psi(B_{\pi_d}) \} + \exp \{ - \sum_{i=1}^n Y_i [T'_{k_1 k_2}^{(i)} + T'_{k_2 k_1}^{(i)}] \}}$$