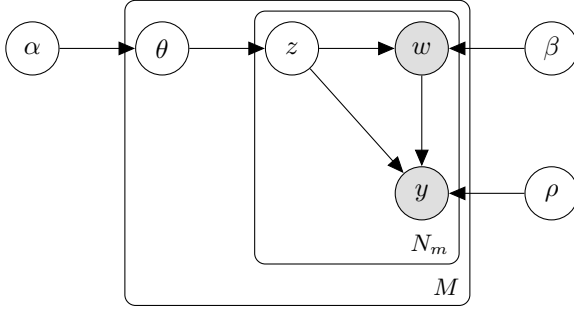
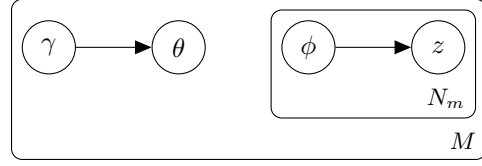


polarLDA

Blue indicates new or additional terms to the original LDA.



(a) The model.



(b) Variational distribution.

1 Generative Process

For patient m ,

1. draw a subtype mixture $\theta \sim \text{Dir}(\alpha)$;
2. for each of his/her N_m voxel involvements, independently
 - (a) draw a subtype $z_n \sim \text{Mult}(\theta)$;
 - (b) draw a voxel $w_n \sim p(w_n \mid z_n, \beta)$;
 - (c) draw an involvement type $y_n \sim p(y_n \mid w_n, z_n, \rho)$.

2 Constructing the Lower Bound

The variational distribution used to approximate the true posterior is factorizable as

$$q(\theta, z \mid \gamma, \phi) = q(\theta \mid \gamma) \prod_{n=1}^N q(z_n \mid \phi_n).$$

The lower bound $\mathcal{L}(\gamma, \phi \mid \alpha, \beta, \rho)$ of the single-brain log-likelihood $\log p(w \mid \alpha, \beta, \rho)$ is computed using Jensen's inequality as follows

$$\begin{aligned}
\log p(w, y \mid \alpha, \beta, \rho) &= \log \int \sum_z p(\theta, z, w, y \mid \alpha, \beta, \rho) d\theta \\
&= \log \int \sum_z \frac{p(\theta, z, w, y \mid \alpha, \beta, \rho) q(\theta, z \mid \gamma, \phi)}{q(\theta, z \mid \gamma, \phi)} d\theta \\
&= \log \int \sum_z q(\theta, z \mid \gamma, \phi) \frac{p(\theta, z, w, y \mid \alpha, \beta, \rho)}{q(\theta, z \mid \gamma, \phi)} d\theta \\
&= \log E_q \left\{ \frac{p(\theta, z, w, y \mid \alpha, \beta, \rho)}{q(\theta, z \mid \gamma, \phi)} \right\} \\
&\geq E_q \{ \log p(\theta, z, w, y \mid \alpha, \beta, \rho) \} - E_q \{ \log q(\theta, z \mid \gamma, \phi) \} \\
&\triangleq \mathcal{L}(\gamma, \phi \mid \alpha, \beta, \rho).
\end{aligned} \tag{1}$$

The difference between the log-likelihood and its lower bound can be proven to be in fact the KL divergence between the variational distribution and the true posterior.

$$\begin{aligned}
&\log p(w, y \mid \alpha, \beta, \rho) - \mathcal{L}(\gamma, \phi \mid \alpha, \beta, \rho) \\
&= E_q \{ \log p(w, y \mid \alpha, \beta, \rho) \} - E_q \{ \log p(\theta, z, w, y \mid \alpha, \beta, \rho) \} + E_q \{ \log q(\theta, z \mid \gamma, \phi) \} \\
&= E_q \left\{ \log \frac{p(w, y \mid \alpha, \beta, \rho) q(\theta, z \mid \gamma, \phi)}{p(\theta, z, w, y \mid \alpha, \beta, \rho)} \right\} \\
&= E_q \left\{ \log \frac{q(\theta, z \mid \gamma, \phi)}{p(\theta, z \mid w, y, \alpha, \beta, \rho)} \right\} \\
&= \text{D}_{\text{KL}}(q(\theta, z \mid \gamma, \phi) \parallel p(\theta, z \mid w, y, \alpha, \beta, \rho)).
\end{aligned}$$

Therefore, maximizing the lower bound is equivalent to minimizing this KL divergence. That is, the variational distribution automatically approaches to the real posterior as we maximize the lower bound.

3 Expanding the Lower Bound

To maximize the lower bound, we first need to spell out the lower bound $\mathcal{L}(\gamma, \phi \mid \alpha, \beta, \rho)$ in terms of the model parameters (α, β, ρ) and the variational parameters (γ, ϕ) . Continuing from (1), we have

$$\begin{aligned}
\mathcal{L}(\gamma, \phi \mid \alpha, \beta) &= E_q \{ \log p(\theta, z, w, y \mid \alpha, \beta, \rho) \} - E_q \{ \log q(\theta, z \mid \gamma, \phi) \} \\
&= E_q \left\{ \log \frac{p(\theta, z, w, y \mid \alpha, \beta, \rho)}{q(\theta, z \mid \gamma, \phi)} \right\} \\
&= E_q \left\{ \log \frac{p(\theta \mid \alpha) p(z \mid \theta) p(w \mid z, \beta) p(y \mid z, w, \rho)}{q(\theta \mid \gamma) q(z \mid \phi)} \right\} \\
&= E_q \{ \log p(\theta \mid \alpha) \} + E_q \{ \log p(z \mid \theta) \} + E_q \{ \log p(w \mid z, \beta) \} \\
&\quad + E_q \{ \log p(y \mid z, w, \rho) \} \\
&\quad - E_q \{ \log q(\theta \mid \gamma) \} - E_q \{ \log q(z \mid \phi) \}.
\end{aligned} \tag{2}$$

We now further expand each of the five terms in (2).

The first term is

$$\begin{aligned}
\mathbb{E}_q \{ \log p(\theta \mid \alpha) \} &= \mathbb{E}_q \left\{ \log \frac{\Gamma \left(\sum_{i=1}^K \alpha_i \right)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \theta_k^{\alpha_k - 1} \right\} \\
&= \mathbb{E}_q \left\{ \log \Gamma \left(\sum_{i=1}^K \alpha_i \right) + \sum_{k=1}^K (\alpha_k - 1) \log \theta_k - \sum_{k=1}^K \log \Gamma(\alpha_k) \right\} \\
&= \sum_{k=1}^K (\alpha_k - 1) \mathbb{E}_q \{ \log \theta_k \} + \log \Gamma \left(\sum_{i=1}^K \alpha_i \right) - \sum_{k=1}^K \log \Gamma(\alpha_k) \\
&= \sum_{k=1}^K (\alpha_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) + \log \Gamma \left(\sum_{i=1}^K \alpha_i \right) - \sum_{k=1}^K \log \Gamma(\alpha_k),
\end{aligned}$$

where $\Psi(\cdot)$ is the digamma function, the first derivative of the log Gamma function. The final line is due to the following property of the Dirichlet distribution as a member of the exponential family. If $\theta \sim \text{Dir}(\alpha)$, then $\mathbb{E}_{p(\theta|\alpha)} \{ \log \theta_i \} = \Psi(\alpha_i) - \Psi(\sum_{i=1}^K \alpha_i)$.

The second term is

$$\begin{aligned}
\mathbb{E}_q \{ \log p(z \mid \theta) \} &= \mathbb{E}_q \left\{ \log \prod_{n=1}^N p(z_n \mid \theta) \right\} \\
&= \mathbb{E}_q \left\{ \log \prod_{n=1}^N \prod_{k=1}^K \theta_k^{\mathbb{1}_z(n,k)} \right\} \\
&= \sum_{n=1}^N \sum_{k=1}^K \mathbb{E}_q \{ \mathbb{1}_z(n, k) \log \theta_k \} \\
&= \sum_{n=1}^N \sum_{k=1}^K \mathbb{E}_q \{ \mathbb{1}_z(n, k) \} \mathbb{E}_q \{ \log \theta_k \} \\
&= \sum_{n=1}^N \sum_{k=1}^K \phi_{nk} \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right),
\end{aligned}$$

where ϕ_{nk} is the probability of the n th voxel being recruited by subtype k , and $\mathbb{1}(\cdot)$ is the indicator function.

We expand **the third term** as

$$\begin{aligned}
\mathbb{E}_q \{ \log p(w \mid z, \beta) \} &= \mathbb{E}_q \left\{ \log \prod_{n=1}^N p(w_n \mid z_n, \beta) \right\} \\
&= \mathbb{E}_q \left\{ \log \prod_{n=1}^N \prod_{k=1}^K \prod_{v=1}^V \beta_{kv}^{\mathbb{1}_z(n,k) \mathbb{1}_w(n,v)} \right\} \\
&= \mathbb{E}_q \left\{ \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \mathbb{1}_z(n, k) \mathbb{1}_w(n, v) \log \beta_{kv} \right\}
\end{aligned}$$

$$\begin{aligned}
&= \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \mathbb{E}_q \{ \mathbb{1}_z(n, k) \} \mathbb{1}_w(n, v) \log \beta_{kv} \\
&= \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) \log \beta_{kv}.
\end{aligned}$$

The fourth (new) term is

$$\begin{aligned}
\mathbb{E}_q \{ \log p(y \mid z, w, \rho) \} &= \mathbb{E}_q \left\{ \log \prod_{n=1}^N p(y_n \mid z_n, w_n, \rho) \right\} \\
&= \mathbb{E}_q \left\{ \log \prod_{n=1}^N \prod_{k=1}^K \prod_{v=1}^V \left(\rho_{kv}^{\mathbb{1}_y(n)} (1 - \rho_{kv})^{1 - \mathbb{1}_y(n)} \right)^{\mathbb{1}_z(n, k) \mathbb{1}_w(n, v)} \right\} \\
&= \mathbb{E}_q \left\{ \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \mathbb{1}_z(n, k) \mathbb{1}_w(n, v) (\mathbb{1}_y(n) \log \rho_{kv} + (1 - \mathbb{1}_y(n)) \log(1 - \rho_{kv})) \right\} \\
&= \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) (\mathbb{1}_y(n) \log \rho_{kv} + (1 - \mathbb{1}_y(n)) \log(1 - \rho_{kv}))
\end{aligned}$$

Very similar to the first term, **the fifth term** is expanded as

$$\mathbb{E}_q \{ \log q(\theta \mid \gamma) \} = \sum_{k=1}^K (\gamma_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) + \log \Gamma \left(\sum_{k=1}^K \gamma_k \right) - \sum_{k=1}^K \log \Gamma(\gamma_k).$$

Finally, **the sixth term** is expanded as

$$\begin{aligned}
\mathbb{E}_q \{ \log q(z \mid \phi) \} &= \mathbb{E}_q \left\{ \log \prod_{n=1}^N q(z_n \mid \phi_n) \right\} \\
&= \mathbb{E}_q \left\{ \log \prod_{n=1}^N \prod_{k=1}^K \phi_{nk}^{\mathbb{1}_z(n, k)} \right\} \\
&= \sum_{n=1}^N \sum_{k=1}^K \mathbb{E}_q \{ \mathbb{1}_z(n, k) \} \log \phi_{nk} \\
&= \sum_{n=1}^N \sum_{k=1}^K \phi_{nk} \log \phi_{nk}.
\end{aligned}$$

Therefore, the fully expanded lower bound is

$$\begin{aligned}
\mathcal{L}(\gamma, \phi \mid \alpha, \beta) &= \sum_{k=1}^K (\alpha_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) + \log \Gamma \left(\sum_{i=1}^K \alpha_i \right) - \sum_{k=1}^K \log \Gamma(\alpha_k) \\
&\quad + \sum_{n=1}^N \sum_{k=1}^K \phi_{nk} \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \\
&\quad + \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) \log \beta_{kv}
\end{aligned} \tag{3}$$

$$\begin{aligned}
& + \sum_{n=1}^N \sum_{k=1}^K \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) (\mathbb{1}_y(n) \log \rho_{kv} + (1 - \mathbb{1}_y(n)) \log(1 - \rho_{kv})) \\
& - \sum_{k=1}^K (\gamma_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) - \log \Gamma \left(\sum_{k=1}^K \gamma_k \right) + \sum_{k=1}^K \log \Gamma(\gamma_k) \\
& - \sum_{n=1}^N \sum_{k=1}^K \phi_{nk} \log \phi_{nk}.
\end{aligned}$$

4 Maximizing the Lower Bound

In this section, we maximize the lower bound w.r.t. the variational parameters ϕ and γ . Recall that as the maximization runs, the KL divergence between the variational distribution and the true posterior drops (E-step of the variational EM algorithm).

4.1 Variational Multinomial

We first maximize Equation (3) w.r.t. ϕ_{nk} . Since $\sum_{k=1}^K \phi_{nk} = 1$, this is a constrained optimization problem that can be solved by the Lagrange multiplier method. The Lagrangian w.r.t. ϕ_{nk} is

$$\begin{aligned}
\mathcal{L}_{[\phi_{nk}]} &= \phi_{nk} \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \\
&+ \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) \log \beta_{kv} \\
&+ \sum_{v=1}^V \phi_{nk} \mathbb{1}_w(n, v) (\mathbb{1}_y(n) \log \rho_{kv} + (1 - \mathbb{1}_y(n)) \log(1 - \rho_{kv})) \\
&- \phi_{nk} \log \phi_{nk} + \lambda_n \left(\sum_{i=1}^K \phi_{ni} - 1 \right),
\end{aligned}$$

where λ_n is the Lagrange multiplier. Taking the derivative, we get

$$\begin{aligned}
\frac{\partial}{\partial \phi_{nk}} \mathcal{L}_{[\phi_{nk}]} &= \Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \\
&+ \sum_{v=1}^V \mathbb{1}_w(n, v) \log \beta_{kv} \\
&+ \sum_{v=1}^V \mathbb{1}_w(n, v) (\mathbb{1}_y(n) \log \rho_{kv} + (1 - \mathbb{1}_y(n)) \log(1 - \rho_{kv})) \\
&- \log \phi_{nk} - 1 + \lambda_n.
\end{aligned}$$

Setting this derivative to zero yields

$$\phi_{nk} = \exp \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) + \lambda_n - 1 \right) \prod_{v=1}^V \left(\beta_{kv} \cdot \rho_{kv}^{\mathbb{1}_y(n)} \cdot (1 - \rho_{kv})^{1 - \mathbb{1}_y(n)} \right)^{\mathbb{1}_w(n, v)}$$

$$\propto \exp \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \prod_{v=1}^V \left(\beta_{kv} \rho_{kv}^{\mathbb{1}_y(n)} \cdot (1 - \rho_{kv})^{1 - \mathbb{1}_y(n)} \right)^{\mathbb{1}_w(n,v)}.$$

4.2 Variational Dirichlet

Now we maximize Equation (3) w.r.t. γ_k , the k th component of the Dirichlet parameter. Only the terms containing γ_k are retained.

$$\begin{aligned} \mathcal{L}_{[\gamma]} &= \sum_{k=1}^K (\alpha_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \\ &+ \sum_{n=1}^N \sum_{k=1}^K \phi_{nk} \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \\ &- \sum_{k=1}^K (\gamma_k - 1) \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) - \log \Gamma \left(\sum_{i=1}^K \gamma_i \right) + \sum_{k=1}^K \log \Gamma(\gamma_k) \end{aligned}$$

Taking the derivative w.r.t. γ_k , we have

$$\begin{aligned} \frac{\partial}{\partial \gamma_k} \mathcal{L}_{[\gamma]} &= \left(\Psi'(\gamma_k) - \Psi' \left(\sum_{i=1}^K \gamma_i \right) \right) (\alpha_k - 1) \\ &+ \left(\Psi'(\gamma_k) - \Psi' \left(\sum_{i=1}^K \gamma_i \right) \right) \sum_{n=1}^N \phi_{nk} \\ &- \left(\Psi'(\gamma_k) - \Psi' \left(\sum_{i=1}^K \gamma_i \right) \right) (\gamma_k - 1) - \left(\Psi(\gamma_k) - \Psi \left(\sum_{i=1}^K \gamma_i \right) \right) \\ &- \frac{\Psi \left(\sum_{i=1}^K \gamma_i \right)}{\Gamma \left(\sum_{i=1}^K \gamma_i \right)} + \frac{\Psi(\gamma_k)}{\Gamma(\gamma_k)} \\ &= \left(\Psi'(\gamma_k) - \Psi' \left(\sum_{i=1}^K \gamma_i \right) \right) \left(\alpha_k + \sum_{n=1}^N \phi_{nk} - \gamma_k \right) - \Psi(\gamma_k) + \Psi \left(\sum_{i=1}^K \gamma_i \right) \\ &- \Psi \left(\sum_{i=1}^K \gamma_i \right) + \Psi(\gamma_k) \\ &= \left(\Psi'(\gamma_k) - \Psi' \left(\sum_{i=1}^K \gamma_i \right) \right) \left(\alpha_k + \sum_{n=1}^N \phi_{nk} - \gamma_k \right). \end{aligned}$$

Setting it to zero, we have

$$\gamma_k = \alpha_k + \sum_{n=1}^N \phi_{nk}.$$

5 Estimating Model Parameters

The previous section is the E-step of the variational EM algorithm, where we tighten the lower bound w.r.t. the variational parameters; this section is the M-step, where we maximize the lower

bound w.r.t. the model parameters α , β , and ρ . Now we add back the document subscript to consider the whole corpus.

By the assumed exchangeability of the documents, the overall log-likelihood of the corpus is just the sum of all the documents' log-likelihoods, and the overall lower bound is just the sum of the individual lower bounds. Again, only the terms involving β are left in the overall lower bound. Adding the Lagrange multipliers, we obtain

$$\mathcal{L}_{[\beta]} = \sum_{m=1}^M \sum_{n=1}^{N_m} \sum_{k=1}^K \sum_{v=1}^V \phi_{mnk} \mathbb{1}_w(m, n, v) \log \beta_{kv} + \sum_{k=1}^K \lambda_k \left(\sum_{v=1}^V \beta_{kv} - 1 \right).$$

Taking the derivative w.r.t. β_{kv} and setting it to zero, we have

$$\begin{aligned} \frac{\partial}{\partial \beta_{kv}} \mathcal{L}_{[\beta]} &= \sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v) \frac{1}{\beta_{kv}} + \lambda_k = 0 \\ \Rightarrow \beta_{kv} &= -\frac{1}{\lambda_k} \sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v) \\ \Rightarrow \beta_{kv} &\propto \sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v). \end{aligned}$$

For α ,

$$\mathcal{L}_{[\alpha]} = \sum_{m=1}^M \left(\sum_{k=1}^K (\alpha_k - 1) \left(\Psi(\gamma_{mk}) - \Psi \left(\sum_{i=1}^K \gamma_{mi} \right) \right) + \log \Gamma \left(\sum_{i=1}^K \alpha_i \right) - \sum_{k=1}^K \log \Gamma(\alpha_k) \right)$$

Assuming a symmetric Dirichlet prior (i.e., $\alpha_k = \alpha, \forall k$), we have

$$\begin{aligned} \mathcal{L}_{[\alpha]} &= \sum_{m=1}^M \left(\sum_{k=1}^K (\alpha - 1) \left(\Psi(\gamma_{mk}) - \Psi \left(\sum_{i=1}^K \gamma_{mi} \right) \right) \right) + M \log \Gamma(K\alpha) - MK \log \Gamma(\alpha) \\ \frac{\partial}{\partial \alpha_k} \mathcal{L}_{[\alpha]} &= \sum_{m=1}^M \sum_{j=1}^K \left(\Psi(\gamma_{mj}) - \Psi \left(\sum_{i=1}^K \gamma_{mi} \right) \right) + MK \Psi(K\alpha) - MK \Psi(\alpha). \end{aligned}$$

Since the derivative also depends on other $\alpha_{k' \neq k}$ in general asymmetric cases, we compute the Hessian

$$\frac{\partial^2}{\partial \alpha_k \partial \alpha_{k'}} \mathcal{L}_{[\alpha]} = MK^2 \Psi'(K\alpha) - MK \Psi'(\alpha),$$

and notice that its form allows for the linear-time Newton-Raphson algorithm.

Finally, for ρ ,

$$\mathcal{L}_{[\rho]} = \sum_{m=1}^M \sum_{n=1}^{N_m} \sum_{k=1}^K \sum_{v=1}^V \phi_{mnk} \mathbb{1}_w(m, n, v) (\mathbb{1}_y(m, n) \log \rho_{kv} + (1 - \mathbb{1}_y(m, n)) \log(1 - \rho_{kv}))$$

Taking the derivative w.r.t. ρ_{kv} and setting it to zero, we have

$$\begin{aligned}
\frac{\partial}{\partial \rho_{kv}} \mathcal{L}_{[\rho]} &= \sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v) \left(\frac{\mathbb{1}_y(m, n)}{\rho_{kv}} - \frac{1 - \mathbb{1}_y(m, n)}{1 - \rho_{kv}} \right) = 0 \\
\Rightarrow \sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v) (\mathbb{1}_y(m, n) - \rho_{kv}) &= 0 \\
\Rightarrow \rho_{kv} &= \frac{\sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v) \mathbb{1}_y(m, n)}{\sum_{m=1}^M \sum_{n=1}^{N_m} \phi_{mnk} \mathbb{1}_w(m, n, v)}.
\end{aligned}$$