

# ALGORITHM FOR PMF BACKGROUND MODEL WITH WEIGHTS

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## 1. Model.

$$(1.1) \quad X_{ij} = \sum_k Z_{ijk}$$

$$(1.2) \quad Z_{ijk} \sim \text{Pois}(w_k l_{i0} f_{j0} l_{ik} f_{jk})$$

$$(1.3) \quad l_{ik} \sim g_{L,k}(\cdot), f_{jk} \sim g_{F,k}(\cdot)$$

We assume that  $X$  is sparse: it has  $m$  nonzero elements and  $m \ll np$ .

## 2. Notation. For $v \sim q(\cdot)$ , I use

$$(2.1) \quad \bar{v} := E_q[v]$$

$$(2.2) \quad \hat{v} := \exp(E_q[\log(v)])$$

And in the algorithm,  $q$  is always the corresponding variational distribution for that variable.

## 3. Algorithm.

### 3.1. ELBO.

$$(3.1) \quad \text{ELBO} = C_1 - C_2 + C_3$$

$$(3.2) \quad C_1 = E[\log p(Z|L, F, L_0, F_0)]$$

$$(3.3) \quad = \sum_{ijk} (-w_k l_{i0} f_{j0} \bar{l}_{ik} \bar{f}_{jk} + \bar{Z}_{ijk} \log(w_k l_{i0} f_{j0} \hat{l}_{ik} \hat{f}_{jk})) - \sum_{ijk} E(\log(Z_{ijk}!))$$

$$(3.4) \quad C_2 = E[\log q_Z(Z)]$$

$$(3.5) \quad = \sum_{ijk} (\bar{Z}_{ijk} \log(\zeta_{ijk})) + \sum_{ij} \log(X_{ij}!) - \sum_{ijk} E(\log(Z_{ijk}!))$$

$$(3.6) \quad C_3 = E(\log \frac{g_L(L)}{q_L(L)} + \log \frac{g_F(F)}{q_F(F)})$$

The last part of  $C_1, C_2$  gets cancelled out.

For convenience, I introduce the following variable:

$$(3.7) \quad B_{ijk} := w_k \hat{l}_{ik} \hat{f}_{jk}$$

$$(3.8) \quad B_{ij} := \sum_k B_{ijk}$$

$$(3.9) \quad \Lambda_{ijk} := w_k \bar{l}_{ik} \bar{f}_{jk}$$

$$(3.10) \quad \Lambda_{ij} := \sum_k \Lambda_{ijk}$$

REMARK. In actual implementation:  $B_{ij}$  is computed and stored only for those where  $X_{ij} \neq 0$ ;  $\Lambda_{ij}$  is not computed nor stored.

### 3.2. Update formula. In iteration $t$

1. update  $\bar{Z}_{ijk}$

Using Lagrange Multiplier on parts relevant to  $\zeta$ , it's easy to see

$$(3.11) \quad \zeta_{ijk} \leftarrow \frac{B_{ijk}}{B_{ij}}$$

$$(3.12) \quad \bar{Z}_{ijk} = X_{ij} \zeta_{ijk}$$

REMARK. *We only need to compute  $\zeta_{ijk}$  where  $X_{ij} \neq 0$ , and we don't need to store this 3 dimensional array. The memory and runtime are only  $O(m)$ , instead of  $O(npK)$ .*

2. update  $q_L, g_L, q_F, g_F$

By observing  $C_1 + C_3$ , we have

$$(3.13) \quad (q_{L,k}, g_{L,k}, \text{kl}_{L,k}) \leftarrow \text{EBPM}(y_i = \bar{Z}_{i,k}, s_i = (\sum_j f_{j0} \bar{f}_{jk}) w_k l_{i0})$$

$$(3.14) \quad (q_{F,k}, g_{F,k}, \text{kl}_{F,k}) \leftarrow \text{EBPM}(y_j = \bar{Z}_{j,k}, s_j = (\sum_i l_{i0} \bar{l}_{ik}) w_k f_{j0})$$

REMARK. *The computation of KL-divergence will be explained later.*

3. update  $B_{ij}$

$$(3.15) \quad B_{ij} = B_{ij} - B_{ijk}^{(t-1)} + B_{ijk}^{(t)}$$

4. update  $l_{i0}, f_{j0}$

Take derivatives in  $C_1$  and use the fact that  $\sum_k \bar{Z}_{ijk} = X_{ij}$ , we have

$$(3.16) \quad l_{i0} \leftarrow \frac{X_{i.}}{\sum_j f_{j0} \Lambda_{ij}} = \frac{X_{i.}}{\sum_k w_k \bar{l}_{ik} (\sum_j f_{j0} \bar{f}_{jk})}$$

$$(3.17) \quad f_{j0} \leftarrow \frac{X_{.j}}{\sum_i l_{i0} \Lambda_{ij}} = \frac{X_{.j}}{\sum_k w_k \bar{f}_{jk} (\sum_i l_{i0} \bar{l}_{ik})}$$

REMARK. *The computation is  $O((n+p)K)$*

5. update  $w_k$

It is easy to see

$$(3.18) \quad w_k \leftarrow \frac{\sum_{ij} \bar{Z}_{ijk}}{\sum_{ij} l_{i0} f_{j0} \bar{l}_{ik} \bar{f}_{jk}}$$

**3.3. ELBO computation after update.** When we plug in the updates into the ELBO, we have

$$(3.19)$$

$$\text{ELBO} = \sum_{ij} (-l_{i0} f_{j0} \Lambda_{ij} + X_{ij} \log(l_{i0} f_{j0} B_{ij}) - \log(X_{ij}!)) + E(\log \frac{g_L(L)}{q_L(L)} + \log \frac{g_F(F)}{q_F(F)})$$

$$(3.20)$$

$$= \sum_{ij} (-l_{i0} f_{j0} \Lambda_{ij} + X_{ij} \log(l_{i0} f_{j0} B_{ij}) - \log(X_{ij}!)) - \sum_k \text{KL}(q_L(l_{Ik}) | g_L(l_{Ik})) - \sum_k \text{KL}(q_F(f_{Jk}) | g_F(f_{Jk}))$$

REMARK. Again, we don't need to compute  $\Lambda$  in actual computation. The KL-divergence will be explained in the next section.

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**Algorithm 3.1** EBPMF-WBG

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Input:  $X_{IJ}, l_{I0}, f_{J0}, q_L, g_L, q_F, g_F, B_{IJ}$

**for**  $t = 1, \dots, T$  **do**

$KL \leftarrow 0$

**for**  $k = 1, \dots, K$  **do**

$B_{ijk} \leftarrow w_k \hat{l}_{ik} \hat{f}_{jk}$

$\bar{Z}_{ijk} \leftarrow X_{ij} \frac{B_{ijk}}{B_{ij}}$

$(q_{L,k}, g_{L,k}, kl_{L,k}) \leftarrow \text{EBPM}(y_i = \bar{Z}_{i,k}, s_i = (\sum_j f_{j0} \bar{f}_{jk}) w_k l_{i0})$

$(q_{F,k}, g_{F,k}, kl_{F,k}) \leftarrow \text{EBPM}(y_j = \bar{Z}_{j,k}, s_j = (\sum_i l_{i0} \bar{l}_{ik}) w_k f_{j0})$

$w_k \leftarrow \frac{\sum_{ij} X_{ij} (B_{ijk} / B_{ij})}{(\sum_i l_{i0} \bar{l}_{ik}) (\sum_j f_{j0} \bar{f}_{jk})}$

$B_{ij} \leftarrow B_{ij} - B_{ijk} + w_k \hat{l}_{ik} \hat{f}_{jk}$

$KL \leftarrow KL + kl_{F,k} + kl_{L,k}$

**end**

$l_{i0} \leftarrow \frac{X_{i.}}{\sum_k w_k \bar{l}_{ik} (\sum_j f_{j0} \bar{f}_{jk})}$

$f_{j0} \leftarrow \frac{X_{.j}}{\sum_k w_k \bar{f}_{jk} (\sum_i l_{i0} \bar{l}_{ik})}$

$\text{ELBO} = \text{compute-elbo}(KL, X, B, \Lambda)$

**end**

Output:  $X_{IJ}, l_{I0}, f_{J0}, q_L, g_L, q_F, g_F$

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### 3.4. Algorithm.

**4. Compute KL divergence from EBPM.** Consider the EBPM problem:

$$(4.1) \quad y_i \sim \text{Pois}(s_i \lambda_i)$$

$$(4.2) \quad \lambda_i \sim g(\cdot)$$

Our procedure optimizes the marginal log-likelihood  $\sum_i \log p(y_i)$  for  $g^*$ , then compute the posterior  $p(\lambda_i | y_i, g^*)$ .

The objective can be re-written this way:

$$(4.3) \quad \sum_i \log p(y_i) = \sum_i \log \frac{p(y_i | \lambda_i) g(\lambda_i)}{p(\lambda_i | y_i)}$$

$$(4.4) \quad = \sum_i E_{q(\lambda_i)} [\log \frac{p(y_i | \lambda_i) g(\lambda_i)}{p(\lambda_i | y_i)}]$$

$$(4.5) \quad = \sum_i E_{q(\lambda_i)} [\log p(y_i | \lambda_i)] - E_{q(\lambda_i)} [\frac{p(\lambda_i | y_i)}{g(\lambda_i)}]$$

Use  $q(\lambda_i) := p(\lambda_i|y_i)$ , we have

$$(4.6) \quad -\text{KL}(p(\boldsymbol{\lambda}|\mathbf{y})|g(\boldsymbol{\lambda})) = \log p(\mathbf{y}) - \sum_i E_{p(\lambda_i|y_i)}[\log p(y_i|\lambda_i)]$$

First term on RHS is given by EBPM; the second term can be easily computed.

**5. Numerical Trick.** Directly computing  $B_{ij}$  has the issue of overflows and underflows.

Let  $a_{ij} := \max_k \log(B_{ijk})$ , and compute the following:

$$(5.1) \quad b_{ijk} := \log(B_{ijk}) - a_{ij}$$

$$(5.2) \quad b_{ij} := \log \sum_k \exp(b_{ijk})$$

We can recover the needed quantities with  $b$ :

$$(5.3) \quad \frac{B_{ijk}}{B_{ij}} = \exp(b_{ijk} - b_{ij})$$

$$(5.4) \quad \log(B_{ij}) = b_{ij} + a_{ij}$$

The advantage of using  $b$  instead of  $B$  is that computing  $\exp(b_{ijk})$  is more numerically stable than computing  $B_{ijk}$ .