

In Gibbs sampling algorithm, the samples are generated from full conditional posteriors of each variable. The full conditional probabilities of variables U, C, L are represented as $p(U|X, C, L), p(C|X, U, L), p(L|X, U, C)$ which are proportional to joint distribution $p(X, U, C, L)$. In each of these probabilities, the intended variable is conditioned on fixed values of other variables and the observation set X . Sampling from these distributions is a hard task in problem. In Metropolis-Hastings algorithm it is not necessary to generate samples from full conditional distributions. Instead a proposal distribution is chosen based on the current value of random variables in a special application. In this case we can use a combination of Gibbs sampling and Metropolis-Hastings algorithms which is called Metropolis-within-Gibbs algorithm. This algorithm which performs the MAP inference to reach the best values of random variables, is represented in algorithm (1).

The proposed distribution for sampling membership values is a Dirichlet distribution using α parameter.

$$u_n^t \sim \text{Dirichlet}(\alpha = 1_S) \quad (1)$$

As mentioned before if we set $\alpha = 1$ the Dirichlet distribution will be symmetric. So the ratio of the proposal density values is equal to 1 and the sampled membership value in time t for data point x_n is evaluated by equation (??) and is accepted with probability a_u which is based on the ratio of target density for proposed and current value.

$$\begin{aligned} p(x_n, u_n | C, L) &= p(x_n | u_n, C, L) \times p(u_n | \alpha) \\ &\propto \prod_{s=1}^S \exp\left\{-\frac{1}{2}(x_n - c_s)^T L^T u_{ns}^m L (x_n - c_s)\right\} \\ &\times \prod_{i=1}^N \exp\left\{-\frac{1}{2} \left(\frac{(u_n \cdot u_i)}{\|u_n\| \|u_i\|} - 0.5 \right) (x_n - x_i)^T L^T L (x_n - x_i)\right\} \times \prod_{s=1}^S u_{ns}^{\alpha_s - 1} \end{aligned} \quad (2)$$

$$a_u = \min\left\{1, \frac{p(x_n, u_n^t | C, L)}{p(x_n, u_n | C, L)}\right\} \quad (3)$$

The proposal distribution for sampling cluster centers is a gaussian distribution

which its mean is the current markov chain state and

$$c_s^t \sim N(c_s, \frac{1}{\delta} \Sigma_x) \quad (4)$$

$$\begin{aligned} \tilde{p}(X, c_s|U, L) &= \tilde{p}(X|U, L, c_s) \times p(c_s|\mu_x, \Sigma_x) \\ &\propto \exp\left\{-\frac{1}{2} \sum_{n=1}^N (x_n - c_s)^T L^T u_{ns}^m L (x_n - c_s)\right\} \\ &\times \exp\left\{-\frac{1}{2} (c_s - \mu_x)^T \Sigma_x^{-1} (c_s - \mu_x)\right\} \end{aligned} \quad (5)$$

$$a_c = \min\left\{1, \frac{p(X, c_s^t|U, L)}{p(X, c_s|U, L)}\right\} \quad (6)$$

$$L_k^t \sim N(0, \text{diag}^{-1}(\nu)) \quad (7)$$

$$\begin{aligned} p(X, L|C, U) &= p(X|C, U, L) \times p(L|\nu) \\ &\propto \exp\left\{-\frac{1}{2} \sum_{n=1}^N \sum_{s=1}^S (x_n - c_s)^T L^T u_{ns}^m L (x_n - c_s)\right\} \\ &\times \exp\left\{-\frac{1}{2} \sum_{n=1}^N \sum_{i=1}^N \left(\frac{(u_n \cdot u_i)}{||u_n|| ||u_i||} - 0.5\right) (x_n - x_i)^T L^T L (x_n - x_i)\right\} \\ &\times \exp\left\{-\frac{1}{2} \sum_{k=1}^p (L_k)^T \text{diag}(\nu) (L_k)\right\} \end{aligned} \quad (8)$$

$$a_L = \min\left\{1, \frac{p(X, L^t|C, U)}{p(X, L|C, U)}\right\} \quad (9)$$

Algorithm 1 Inference algorithm for GBML model

Input: Data matrix X , fuzzifier m , Dirichlet parameter α , number of clusters S ;

Gamma hyperparameters a and b , number of sampling iterations N_{iter} ;

Output: MAP estimates for membership values U^* , cluster centers C^* and transformation matrix L^* ;

- 1: initialize hyperparameters a^*, b^*, α and set μ_x, Σ_x according to (??) and (??);
- 2: sample initial $u_n \sim \text{Dirichlet}(\alpha = 1_S)$ for all $n = \{1, \dots, N\}$;
- 3: sample initial $c_s \sim N(\mu_x, \Sigma_x)$ for all $s = \{1, \dots, S\}$;
- 4: sample initial $L = I_p$;
- 5: set MAP samples to current states $u_n^* \leftarrow u_n, c_s^* \leftarrow c_s, L_k^* \leftarrow L_k$ for all $n = \{1, \dots, N\}, s = \{1, \dots, S\}, k = \{1, \dots, p\}$
- 6: **for** $iter = 1 \dots N_{iter}$ **do**
- 7: /* Sample $U \sim p(U|X, C, L) \propto p(X, C, U, L)$ */
- 8: **for** $n = \{1, \dots, N\}$ **do**
- 9: sample proposed new membership vector u_n^t from ()
- 10: accept $(u_n \leftarrow u_n^t)$ proposal with probability a_u from ()
- 11: **if** $p(x_n, u_n^t | C^*, L^*) > p(x_n, u_n^* | C^*, L^*)$ using () **then**
- 12: $u_n^* \leftarrow u_n^t$
- 13: /* Sample $C \sim p(C|X, U, L) \propto p(X, C, U, L)$ */
- 14: **for** $s = \{1, \dots, S\}$ **do**
- 15: sample proposed new cluster center c_s^t from ()
- 16: accept proposal $(c_s \leftarrow c_s^t)$ with probability a_c from ()
- 17: **if** $p(X, c_s^t | U^*, L^*) > p(X, c_s^* | U^*, L^*)$ using () **then**
- 18: $c_s^* \leftarrow c_s^t$
- 19: /* Sample $L \sim p(L|X, C, U) \propto p(X, C, U, L)$ */
- 20: **for** $k = \{1, \dots, p\}$ **do**
- 21: sample proposed new cluster center L_k^t from ()
- 22: **for** $q = \{1, \dots, p\}$ **do**
- 23: **if** $q == k$ **then** $L_q^t = L_k^t$
- 24: accept proposal $(L_k \leftarrow L_k^t)$ with probability a_L from ()
- 25: **if** $p(X, L_k^t | C^*, U^*) > p(X, L_k^* | C^*, U^*)$ using () **then**
- 26: $L_k^* \leftarrow L_k^t$
- 27: /* check full sample for new maximum likelihood */
- 28: **if** $p(X, C, U, L) > p(X, C^*, U^*, L^*)$ using () **then**
- 29: $U^* \leftarrow U$
- 30: $C^* \leftarrow C$