

$$\begin{bmatrix} X^1 \\ \vdots \\ X^m \end{bmatrix} = \alpha \begin{bmatrix} A_1 \times B^1 \\ \vdots \\ A_n \times B^1 \\ \vdots \\ A_1 \times B^m \\ \vdots \\ A_n \times B^m \end{bmatrix} \begin{bmatrix} X^1 \\ \vdots \\ X^m \end{bmatrix} + (1-\alpha) \begin{bmatrix} X^{10} \\ \vdots \\ X^{m0} \end{bmatrix} \quad (4)$$

Let  $C$  denote  $\begin{bmatrix} A_1 \times B^1 & \cdots & A_n \times B^1 & \cdots & A_1 \times B^n & \cdots & A_n \times B^m \end{bmatrix}^T$  and  $i = sn + t$ ,  $j = rn + \theta$ ,  $s = sI\{t > 0\} + (s-1)I\{t = 0\}$ ,  $t = tI\{t > 0\} + nI\{t = 0\}$ ,  $r = rI\{\theta > 0\} + (r-1)I\{\theta = 0\}$ ,  $\theta = \theta I\{\theta > 0\} + nI\{\theta = 0\}$ ,  $0 \leq t, \theta < n$ .

Then we get:  $c_{i,j} = a_{t,\theta} b_{r+1,s+1}$  and  $c_{j,i} = a_{\theta,t} b_{s+1,r+1}$ .

By comparing the above two equations, we can easily find that  $C$  is a symmetrical matrix with row and column number  $n \times m$ . If we use  $X^*$  to represents  $\begin{bmatrix} X^1 & \cdots & X^n \end{bmatrix}^T$ , then equation (4) can also be written as:

$$X^* = \alpha C X^* + (1-\alpha) X^{*0} \quad (5)$$

According to (Vanunu, et al. 2010)<sup>29</sup>, in order to get a converged solution for equation (5),  $C$  is normalized as:  $C^{norm} = D^{-1/2} C D^{-1/2}$ , where  $D$  is diagonal matrix with  $d_{i,i}$  equals to the sum of the  $i$ -th row of  $C$ . Therefore, we

also have  $c_{i,j}^{norm} = \frac{c_{i,j}}{\sqrt{d_{i,i} d_{j,j}}}$  and  $d_{i,i} = \sum_{u=1}^{nm} c_{i,u} = \sum_{u=1}^{nm} a_{t,\theta_u} b_{r_u+1,s+1} = \sum_{p=1}^n a_{t,p} \sum_{q=1}^m b_{q,s+1}$

where  $u = r_u n + \theta_u$ . By incorporating the above equation into  $c_{i,j}^{norm}$ , we can get

$$c_{i,j}^{norm} = \frac{a_{t,\theta} b_{r+1,s+1}}{\sqrt{\sum_{p=1}^n a_{t,p} \sum_{q=1}^m b_{q,s+1}} \sqrt{\sum_{p=1}^n a_{\theta,p} \sum_{q=1}^m b_{q,r+1}}} = \frac{a_{t,\theta}}{\sqrt{\sum_{p=1}^n a_{t,p} \sum_{p=1}^n a_{\theta,p}}} \frac{b_{r+1,s+1}}{\sqrt{\sum_{q=1}^m b_{q,s+1} \sum_{q=1}^m b_{q,r+1}}}$$

Therefore, if we normalize  $A$  and  $B$  as  $a_{i,j}^{norm} = \frac{a_{i,j}}{\sqrt{\sum_{p=1}^n a_{i,p} \sum_{p=1}^n a_{j,p}}}$  and  $b_{i,j}^{norm} = \frac{b_{i,j}}{\sqrt{\sum_{q=1}^m b_{q,i} \sum_{q=1}^m b_{q,j}}}$

We can get  $c_{i,j}^{norm} = a_{t,\theta}^{norm} b_{r+1,s+1}^{norm}$ .

With this equation, we can rewrite equation (5) as  $X^* = \alpha C^{norm} X^* + (1-\alpha) X^{*0}$

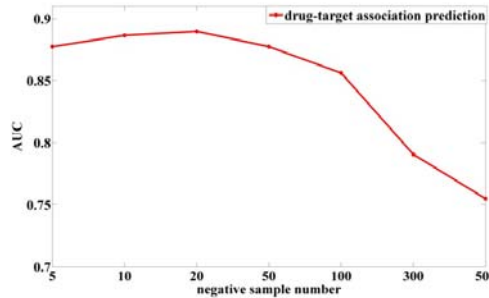


Figure S1 Cross-validation results of BLM using different numbers of negative samples.