

# Alternating-direction-method of Multipliers-Based Adaptive Nonnegative Latent Factor Analysis: Supplementary Materials

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This is the supplementary file for the paper entitled *Alternating-direction-method of Multipliers-Based Adaptive Nonnegative Latent Factor Analysis*. Detailed convergence proof of A<sup>2</sup>NLF and additional figures are presented here.

## I. CONVERGENCE OF A<sup>2</sup>NLF

### A. Proof of Lemma 1

Note that learning objective of A<sup>2</sup>NLF-PSO/A<sup>2</sup>NLF-TPE is non-convex. According to [48], any of its limit points where the gradient becomes zero can be a local/global optimum, or saddle point. Hence, such a limit point can be treated as a solution. Supposing that the optimal solution to  $a_{u,k(q)}$  by (4c) is  $a'_{u,k(q)}$ . Thus, it fulfills the following condition:

$$\lambda'_{(q)} |\Lambda(u)| \left( p'_{u,k(q)} - a'_{u,k(q)} + \frac{h'_{u,k(q)}{}^{t-1}}{\lambda'_{(q)} |\Lambda(u)|} \right) = 0. \quad (S1)$$

Following (4e) and (5c), by applying the update rule of  $h_{u,k(q)}$  to (S1), we have:

$$h'_{u,k(q)} = (\eta'_{(q)} - 1) \lambda'_{(q)} |\Lambda(u)| (p'_{u,k(q)} - a'_{u,k(q)}). \quad (S2)$$

Then (22a) stands based on (S2). Following the same principle, we can derive the optimality condition of (5b) related to  $x_{i,k(q)}$ :

$$\lambda'_{(q)} |\Lambda(i)| \left( z'_{i,k(q)} - x'_{i,k(q)} + \frac{w'_{i,k(q)}{}^{t-1}}{\lambda'_{(q)} |\Lambda(i)|} \right) = 0, \Rightarrow w'_{i,k(q)} = (\eta'_{(q)} - 1) \lambda'_{(q)} |\Lambda(i)| (z'_{i,k(q)} - x'_{i,k(q)}). \quad (S3)$$

Then (22b) holds based on (S3). Hence, *Lemma 1* holds, and **Step 1** is implemented.□

### B. Proof of Lemma 2

Considering the difference between  $g(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'^{t-1}_{2(q)})$  and  $g(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)})$ , we have:

$$\begin{aligned} & g(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'^{t-1}_{2(q)}) - g(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)}) \\ &= \left( \sum_{i \in \Lambda(u)} z'^{t-1}_{i,k(q)} \left( y_{u,i} - \sum_{l_1=1}^{k-1} p'_{u,l_1(q)} z'_{i,l_1(q)} - p'_{u,k(q)} z'_{i,k(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right) - \lambda'_{(q)} |\Lambda(u)| \left( p'_{u,k(q)} - a'^{t-1}_{u,k(q)} + \frac{h'_{u,k(q)}{}^{t-1}}{\lambda'_{(q)} |\Lambda(u)|} \right) \right) (p'^{t-1}_{u,k(q)} - p'_{u,k(q)}) \\ &+ \left( \sum_{u \in \Lambda(i)} p'^{t-1}_{u,k(q)} \left( y_{u,i} - \sum_{l_1=1}^{k-1} p'_{u,l_1(q)} z'_{i,l_1(q)} - p'^{t-1}_{u,k(q)} z'_{i,k(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right) - \lambda'_{(q)} |\Lambda(i)| \left( z'_{i,k(q)} - x'^{t-1}_{i,k(q)} + \frac{w'_{i,k(q)}{}^{t-1}}{\lambda'_{(q)} |\Lambda(i)|} \right) \right) (z'^{t-1}_{i,k(q)} - z'_{i,k(q)}) \\ &- \frac{1}{2} \left( \sum_{i \in \Lambda(u)} (z'^{t-1}_{i,k(q)})^2 + \lambda'_{(q)} |\Lambda(u)| \right) (p'_{u,k(q)} - p'^{t-1}_{u,k(q)})^2 - \frac{1}{2} \left( \sum_{u \in \Lambda(i)} (p'^{t-1}_{u,k(q)})^2 + \lambda'_{(q)} |\Lambda(i)| \right) (z'_{i,k(q)} - z'^{t-1}_{i,k(q)})^2. \end{aligned} \quad (S4)$$

where (\*) performs the second-order Taylor expansion of the left term. Then, considering (5a)'s optimality condition, (S4) is

transformed as:

$$\begin{aligned} & g\left(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'^{t-1}_{2(q)}\right) - g\left(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)}\right) \\ &= -\frac{1}{2} \left( \sum_{i \in \Lambda(u)} \left( z'^{t-1}_{i,k(q)} \right)^2 + \lambda'_{(q)} |\Lambda(u)| \right) \left( p'_{u,k(q)} - p'^{t-1}_{u,k(q)} \right)^2 - \frac{1}{2} \left( \sum_{u \in \Lambda(i)} \left( p'^{t-1}_{u,k(q)} \right)^2 + \lambda'_{(q)} |\Lambda(i)| \right) \left( z'_{i,k(q)} - z'^{t-1}_{i,k(q)} \right)^2. \end{aligned} \quad (S5)$$

Thus, the difference between  $g\left(\psi'^t_{1(q)}, \psi'^{t-1}_{2(q)}\right)$  and  $g\left(p'^t_{u,k(q)}, z'^t_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'^{t-1}_{2(q)}\right)$  is:

$$g\left(\psi'^t_{1(q)}, \psi'^{t-1}_{2(q)}\right) - g\left(p'^t_{u,k(q)}, z'^t_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'^{t-1}_{2(q)}\right) = -\left(\lambda'_{(q)} |\Lambda(u)|/2\right) \left(a'^t_{u,k(q)} - a'^{t-1}_{u,k(q)}\right)^2 - \left(\lambda'_{(q)} |\Lambda(i)|/2\right) \left(x'^t_{i,k(q)} - x'^{t-1}_{i,k(q)}\right)^2. \quad (S6)$$

Moreover,  $g\left(\psi'^t_{1(q)}, \psi'^t_{2(q)}\right)$  and  $g\left(\psi'^t_{1(q)}, \psi'^{t-1}_{2(q)}\right)$  yields:

$$\begin{aligned} & g\left(\psi'^t_{1(q)}, \psi'^t_{2(q)}\right) - g\left(\psi'^t_{1(q)}, \psi'^{t-1}_{2(q)}\right) \\ &= \left(p'^t_{u,k(q)} - a'^t_{u,k(q)}\right) \left(h'^t_{u,k(q)} - h'^{t-1}_{u,k(q)}\right) + \left(z'^t_{i,k(q)} - x'^t_{i,k(q)}\right) \left(w'^t_{i,k(q)} - w'^{t-1}_{i,k(q)}\right) \\ &\stackrel{(I)}{=} \frac{1}{\eta'_{(q)} \lambda'_{(q)} |\Lambda(u)|} \left(h'^t_{u,k(q)} - h'^{t-1}_{u,k(q)}\right)^2 + \frac{1}{\eta'_{(q)} \lambda'_{(q)} |\Lambda(i)|} \left(w'^t_{i,k(q)} - w'^{t-1}_{i,k(q)}\right)^2 \\ &\stackrel{(II)}{\leq} \frac{2|\Lambda(u)|}{\eta'_{(q)} \lambda'_{(q)}} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} p'^t_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} p'^{t-1}_{u,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} a'^t_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} a'^{t-1}_{u,k(q)} \right)^2 \right) \\ &+ \frac{2|\Lambda(i)|}{\eta'_{(q)} \lambda'_{(q)}} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} z'^t_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} z'^{t-1}_{i,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} x'^t_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} x'^{t-1}_{i,k(q)} \right)^2 \right), \end{aligned} \quad (S7)$$

where (I) is based on the update rules of  $(h_{u,k(q)}, w_{i,k(q)})$  given in (4e), (4f) and (5c), and (II) is achieved with *Lemma 1*. With (S5)-(S7), we have the following deduction:

$$\begin{aligned} & g\left(\psi'^t_{1(q)}, \psi'^t_{2(q)}\right) - g\left(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)}\right) \\ &\leq -\frac{1}{2} \left( \sum_{i \in \Lambda(u)} \left( z'^{t-1}_{i,k(q)} \right)^2 + \lambda'_{(q)} |\Lambda(u)| \right) \left( p'^t_{u,k(q)} - p'^{t-1}_{u,k(q)} \right)^2 - \frac{\lambda'_{(q)} |\Lambda(u)|}{2} \left( a'^t_{u,k(q)} - a'^{t-1}_{u,k(q)} \right)^2 \\ &- \frac{1}{2} \left( \sum_{u \in \Lambda(i)} \left( p'^{t-1}_{u,k(q)} \right)^2 + \lambda'_{(q)} |\Lambda(i)| \right) \left( z'^t_{i,k(q)} - z'^{t-1}_{i,k(q)} \right)^2 - \frac{\lambda'_{(q)} |\Lambda(i)|}{2} \left( x'^t_{i,k(q)} - x'^{t-1}_{i,k(q)} \right)^2 \\ &+ \frac{2|\Lambda(u)|}{\eta'_{(q)} \lambda'_{(q)}} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} p'^t_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} p'^{t-1}_{u,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} a'^t_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} a'^{t-1}_{u,k(q)} \right)^2 \right) \\ &+ \frac{2|\Lambda(i)|}{\eta'_{(q)} \lambda'_{(q)}} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} z'^t_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} z'^{t-1}_{i,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} x'^t_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} x'^{t-1}_{i,k(q)} \right)^2 \right). \end{aligned} \quad (S8)$$

Owing to (24a), (25a) stands, which indicates that the augmented Lagrangian function (3) related to  $s_{(q)}$  or  $\tau_q$  is non-increasing as  $a'_{u,k(q)} > 0$  and  $\lambda'_{i,k(q)} > 0$ . Then after the  $t$ -th iteration, the partial objective from (3) related to  $s_{(q)}$  or  $\tau_q$  is formulated as:

$$\begin{aligned} & g\left(\psi'^t_{1(q)}, \psi'^t_{2(q)}\right) \\ &= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left( y_{u,i} - \sum_{l_1=1}^k p'_{u,l_1(q)} z'_{i,l_1(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right)^2 \\ &+ \sum_u \left( \left( \sum_{l_1=1}^k h'_{u,l_1(q)} \left( p'_{u,l_1(q)} - a'^t_{u,l_1(q)} \right) \right) + \left( \sum_{l_2=k+1}^d h'^{t-1}_{u,l_2(q)} \left( p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)} \right) \right) \right) + \sum_i \left( \left( \sum_{l_1=1}^k w'_{i,l_1(q)} \left( z'_{i,l_1(q)} - x'^t_{i,l_1(q)} \right) \right) + \left( \sum_{l_2=k+1}^d w'^{t-1}_{i,l_2(q)} \left( z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)} \right) \right) \right) \\ &+ \sum_u \frac{\lambda'_{(q)} |\Lambda(u)|}{2} \left( \sum_{l_1=1}^k \left( p'_{u,l_1(q)} - a'^t_{u,l_1(q)} \right)^2 + \sum_{l_2=k+1}^d \left( p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)} \right)^2 \right) + \sum_i \frac{\lambda'_{(q)} |\Lambda(i)|}{2} \left( \sum_{l_1=1}^k \left( z'_{i,l_1(q)} - x'^t_{i,l_1(q)} \right)^2 + \sum_{l_2=k+1}^d \left( z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)} \right)^2 \right). \end{aligned}$$

(S9)

By substituting (S2) and (S3) into (S9), we have:

$$\begin{aligned}
& g(\psi'_{1(q)}, \psi'_{2(q)}) \\
&= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left( y_{u,i} - \sum_{l_1=1}^k p'_{u,l_1(q)} z'_{i,l_1(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right)^2 \\
&+ \sum_u |\Lambda(u)| \left( (\eta'_{(q)} - 1) \lambda'_{(q)} \sum_{l_1=1}^k (p'_{u,l_1(q)} - a'_{u,l_1(q)})^2 + (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} \sum_{l_2=k+1}^d (p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)})^2 \right) \\
&+ \sum_i |\Lambda(i)| \left( (\eta'_{(q)} - 1) \lambda'_{(q)} \sum_{l_1=1}^k (z'_{i,l_1(q)} - x'_{i,l_1(q)})^2 + (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} \sum_{l_2=k+1}^d w'_{i,l_2(q)} (z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)})^2 \right) \\
&+ \sum_u \frac{\lambda'_{(q)} |\Lambda(u)|}{2} \left( \sum_{l_1=1}^k (p'_{u,l_1(q)} - a'_{u,l_1(q)})^2 + \sum_{l_2=k+1}^d (p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)})^2 \right) + \sum_i \frac{\lambda'_{(q)} |\Lambda(i)|}{2} \left( \sum_{l_1=1}^k (z'_{i,l_1(q)} - x'_{i,l_1(q)})^2 + \sum_{l_2=k+1}^d (z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)})^2 \right).
\end{aligned} \tag{S10}$$

(S10) indicates that if (24b) is fulfilled, (25b) holds, thereby making (3) related to  $s_{(q)}$  or  $\tau_q$  lower-bounded as  $a'_{u,k(q)} > 0$  and  $x'_{i,k(q)} > 0$ . Based on the above inferences, *Lemma 2* stands, and **Step 2** is implemented.  $\square$

### C. Proof of Theorem 1

**Part a.** Following *Lemma 2*,  $g(\psi'_{1(q)}, \psi'_{2(q)})$  converges as  $t \rightarrow \infty$ , indicating that:

$$\lim_{t \rightarrow \infty} g(\psi'_{1(q)}, \psi'_{2(q)}) - g(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)}) \rightarrow 0. \tag{S11}$$

With (24), when (S1) is fulfilled, the upper-bound of  $g(\psi'_{1(q)}, \psi'_{2(q)}) - g(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)})$  is zero as  $t \rightarrow \infty$ , thereby achieving (26). Following (S8) and (26), we have [24]:

$$\lim_{t \rightarrow \infty} (p'_{u,k(q)} - p'^{t-1}_{u,k(q)}) \rightarrow 0, \tag{S12a}$$

$$\lim_{t \rightarrow \infty} (z'_{i,k(q)} - z'^{t-1}_{i,k(q)}) \rightarrow 0, \tag{S12b}$$

$$\lim_{t \rightarrow \infty} (a'_{u,k(q)} - a'^{t-1}_{u,k(q)}) \rightarrow 0, \tag{S12c}$$

$$\lim_{t \rightarrow \infty} (x'_{i,k(q)} - x'^{t-1}_{i,k(q)}) \rightarrow 0, \tag{S12d}$$

$$\lim_{t \rightarrow \infty} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} p'_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} p'^{t-1}_{u,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} a'_{u,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} a'^{t-1}_{u,k(q)} \right)^2 \right) \rightarrow 0, \tag{S12e}$$

$$\lim_{t \rightarrow \infty} \left( \left( (\eta'_{(q)} - 1) \lambda'_{(q)} z'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} z'^{t-1}_{i,k(q)} \right)^2 + \left( (\eta'_{(q)} - 1) \lambda'_{(q)} x'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} x'^{t-1}_{i,k(q)} \right)^2 \right) \rightarrow 0. \tag{S12f}$$

Based on (22) and (S12), we have the following inferences:

$$\lim_{t \rightarrow \infty} (h'_{u,k(q)} - h'^{t-1}_{u,k(q)}) \rightarrow 0, \tag{S13a}$$

$$\lim_{t \rightarrow \infty} (w'_{i,k(q)} - w'^{t-1}_{i,k(q)}) \rightarrow 0. \tag{S13b}$$

Based on (4e), (4f) and (S13), we conclude that (27) is fulfilled.

**Part b.** Firstly, following (4a), (4b) and (5a), the update rules of  $(p_{u,k(q)}, z_{i,k(q)})$  can be rearranged as:

$$\left(p_{u,k(q)}^{t-1} - p_{u,k(q)}^t\right) \left( \sum_{i \in \Lambda(u)} \left(z_{i,k(q)}^{t-1}\right)^2 + \lambda_{(q)}^t |\Lambda(u)| \right) \quad (\text{S14a})$$

$$= \sum_{i \in \Lambda(u)} z_{i,k(q)}^{t-1} \left( \sum_{l_1=1}^k p_{u,l_1(q)}^t z_{i,l_1(q)}^t + \sum_{l_2=k+1}^d p_{u,l_2(q)}^{t-1} z_{i,l_2(q)}^{t-1} - y_{u,i} \right) + \lambda_{(q)}^t |\Lambda(u)| \left( p_{u,k(q)}^{t-1} - a_{u,k(q)}^{t-1} \right) + h_{u,k(q)}^{t-1},$$

$$\left(z_{i,k(q)}^{t-1} - z_{i,k(q)}^t\right) \left( \sum_{u \in \Lambda(i)} \left(p_{i,k(q)}^{t-1}\right)^2 + \lambda_{(q)}^t |\Lambda(i)| \right) \quad (\text{S14b})$$

$$= \sum_{u \in \Lambda(i)} p_{u,k(q)}^{t-1} \left( \sum_{l_1=1}^k p_{u,l_1(q)}^t z_{i,l_1(q)}^t + \sum_{l_2=k+1}^d p_{u,l_2(q)}^{t-1} z_{i,l_2(q)}^{t-1} - y_{u,i} \right) + \lambda_{(q)}^t |\Lambda(i)| \left( z_{i,k(q)}^{t-1} - x_{i,k(q)}^{t-1} \right) + w_{i,k(q)}^{t-1}.$$

Then by substituting (27) and (S12) into (S14), we have:

$$\sum_{i \in \Lambda(u)} z_{i,k(q)}^{t-1} \left( \sum_{l_1=1}^k p_{u,l_1(q)}^t z_{i,l_1(q)}^t + \sum_{l_2=k+1}^d p_{u,l_2(q)}^{t-1} z_{i,l_2(q)}^{t-1} - y_{u,i} \right) + h_{u,k(q)}^{t-1} \rightarrow 0, \quad (\text{S15a})$$

$$\sum_{u \in \Lambda(i)} p_{u,k(q)}^{t-1} \left( \sum_{l_1=1}^k p_{u,l_1(q)}^t z_{i,l_1(q)}^t + \sum_{l_2=k+1}^d p_{u,l_2(q)}^{t-1} z_{i,l_2(q)}^{t-1} - y_{u,i} \right) + w_{i,k(q)}^{t-1} \rightarrow 0. \quad (\text{S15b})$$

Hence, considering a limit point  $\{\psi_{1(q)}^*, \psi_{2(q)}^*\}$  of a sequence  $\{\psi_{1(q)}^t, \psi_{2(q)}^t\}$  generated by the update rules of  $\{\psi_{1(q)}, \psi_{2(q)}\}$  based on (4) and (5), the following KKT conditions are satisfied with (27) and (S15):

$$\sum_{i \in \Lambda(u)} z_{i,k(q)}^* \left( \sum_{k=1}^d p_{u,k(q)}^* z_{i,k(q)}^* - y_{u,i} \right) + h_{u,k(q)}^* \rightarrow 0, \quad (\text{S16a})$$

$$\sum_{u \in \Lambda(i)} p_{u,k(q)}^* \left( \sum_{k=1}^d p_{u,k(q)}^* z_{i,k(q)}^* - y_{u,i} \right) + w_{i,k(q)}^* \rightarrow 0, \quad (\text{S16b})$$

$$p_{u,k}^* - a_{u,k}^* \rightarrow 0, \quad (\text{S16c})$$

$$z_{i,k}^* - x_{i,k}^* \rightarrow 0. \quad (\text{S16d})$$

Afterwards, considering the remaining KKT conditions regarding constraints  $a_{u,k(q)} > 0$  and  $x_{i,k(q)} > 0$ , we extend the original augmented Lagrangian g:

$$g_{(q)}^{\#} = g_{(q)} - \text{Tr} \left( M_{(q)} \left( A_{(q)} \right)^T \right) - \text{Tr} \left( N_{(q)} \left( X_{(q)} \right)^T \right) = g_{(q)} - \sum_{(u,k)} m_{u,k(q)} a_{u,k(q)} - \sum_{(i,k)} n_{i,k(q)} x_{i,k(q)}, \quad (\text{S17})$$

where the operator  $\text{Tr}(\cdot)$  computes the trace of an enclosed matrix, and the definition of  $g_{(q)}$  is given by:

$$g_{(q)} = \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left( y_{u,i} - \sum_{k=1}^d p_{u,k(q)} z_{i,k(q)} \right)^2 + \sum_{(u,k)} h_{u,k(q)} \left( p_{u,k(q)} - a_{u,k(q)} \right) + \sum_{(u,k)} \frac{\lambda_{(q)} |\Lambda(u)|}{2} \left( p_{u,k(q)} - a_{u,k(q)} \right)^2 \quad (\text{S18})$$

$$+ \sum_{(i,k)} w_{i,k(q)} \left( z_{i,k(q)} - x_{i,k(q)} \right) + \sum_{(i,k)} \frac{\lambda_{(q)} |\Lambda(i)|}{2} \left( z_{i,k(q)} - x_{i,k(q)} \right)^2.$$

For the partial derivatives of  $g_{(q)}^{\#}$  with  $a_{u,k(q)}$  and  $x_{i,k(q)}$ , we have:

$$\begin{cases} \frac{\partial g_{(q)}^\#}{\partial a_{u,k}} = -\lambda_{(q)} |\Lambda(u)| \left( p_{u,k(q)} - a_{u,k(q)} + \frac{h_{u,k(q)}}{\lambda_{(q)} |\Lambda(u)|} \right) - m_{u,k(q)} = 0, \\ \frac{\partial g_{(q)}^\#}{\partial x_{i,k}} = -\lambda_{(q)} |\Lambda(i)| \left( z_{i,k(q)} - x_{i,k(q)} + \frac{w_{i,k(q)}}{\lambda_{(q)} |\Lambda(i)|} \right) - n_{i,k(q)} = 0, \end{cases} \Rightarrow \begin{cases} m_{u,k} = -\lambda_{(q)} |\Lambda(u)| \left( p_{u,k(q)} - a_{u,k(q)} + \frac{h_{u,k(q)}}{\lambda_{(q)} |\Lambda(u)|} \right), \\ n_{i,k} = -\lambda_{(q)} |\Lambda(i)| \left( z_{i,k(q)} - x_{i,k(q)} + \frac{w_{i,k(q)}}{\lambda_{(q)} |\Lambda(i)|} \right). \end{cases} \quad (\text{S19})$$

Then, with the KKT conditions of  $\forall m_{u,k(q)}, a_{u,k(q)}: m_{u,k(q)} a_{u,k(q)} = 0$  and  $\forall n_{i,k(q)}, x_{i,k(q)}: n_{i,k(q)} x_{i,k(q)} = 0$  for (S17), we achieve the following equations based on (S19) [19, 21, 24, 39]:

$$\begin{cases} a_{u,k(q)} \left( -\lambda_{(q)} |\Lambda(u)| \left( p_{u,k(q)} - a_{u,k(q)} + \frac{h_{u,k(q)}}{\lambda_{(q)} |\Lambda(u)|} \right) \right) = 0, \\ x_{i,k(q)} \left( -\lambda_{(q)} |\Lambda(i)| \left( z_{i,k(q)} - x_{i,k(q)} + \frac{w_{i,k(q)}}{\lambda_{(q)} |\Lambda(i)|} \right) \right) = 0, \end{cases} \Rightarrow \begin{cases} a_{u,k(q)} = p_{u,k(q)} + \frac{h_{u,k(q)}}{\lambda_{(q)} |\Lambda(u)|}, \\ x_{i,k(q)} = z_{i,k(q)} + \frac{w_{i,k(q)}}{\lambda_{(q)} |\Lambda(i)|}. \end{cases} \quad (\text{S20})$$

To satisfy the nonnegativity of output LFs  $a_{u,k(q)}$  and  $x_{i,k(q)}$ , (S20) can be rewritten as:

$$\begin{cases} a_{u,k(q)} = \max \left( 0, p_{u,k(q)} + \frac{h_{u,k(q)}}{\lambda_{(q)} |\Lambda(u)|} \right), \\ x_{i,k(q)} = \max \left( 0, z_{i,k(q)} + \frac{w_{i,k(q)}}{\lambda_{(q)} |\Lambda(i)|} \right). \end{cases} \quad (\text{S21})$$

Note that (S21) is consistent with the update rules of  $a_{u,k(q)}$  and  $x_{i,k(q)}$  based on (4c) and (4d). Therefore, (S17)-(S21) show that learning rules of A<sup>2</sup>NLF-PSO/A<sup>2</sup>NLF-TPE are closely connected with the KKT conditions of its learning objective.

Then considering the KKT conditions related to  $a_{u,k(q)}$ :

$$\left. \frac{\partial g_{(q)}^\#}{\partial a_{u,k(q)}} \right|_{a_{u,k(q)} = a_{u,k(q)}^*} = -\lambda_{(q)}^* |\Lambda(u)| \left( p_{u,k(q)}^* - a_{u,k(q)}^* + \frac{h_{u,k(q)}^*}{\lambda_{(q)}^* |\Lambda(u)|} \right) - m_{u,k(q)}^* = 0, \quad (\text{S22a})$$

$$m_{u,k(q)}^* a_{u,k(q)}^* = 0, \quad (\text{S22b})$$

$$a_{u,k(q)}^* \geq 0, \quad (\text{S22c})$$

$$m_{u,k(q)}^* \geq 0, \quad (\text{S22d})$$

where  $a_{u,k(q)}^*$  is a KKT stationary point of  $a_{u,k(q)}$ , and  $m_{u,k(q)}^*$  is a limit point of the sequence  $\{m_{u,k(q)}^t\}$  generated by the update rules of  $m_{u,k}$  based on (S19). According to (S17)-(S21) and  $a_{u,k(q)}^t = 0$ , conditions (S22a)-(S22c) are satisfied. Thus, we have:

$$m_{u,k(q)}^* = -\lambda_{(q)}^* |\Lambda(u)| \left( p_{u,k(q)}^* - a_{u,k(q)}^* + \frac{h_{u,k(q)}^*}{\lambda_{(q)}^* |\Lambda(u)|} \right). \quad (\text{S23})$$

Thus, we focus on condition (S22d). Since  $a_{u,k(q)}^t > 0$  in this case, the update rule for  $a_{u,k(q)}$  is given as:

$$a_{u,k(q)}^* \leftarrow p_{u,k(q)}^* + \frac{h_{u,k(q)}^*}{\lambda_{(q)}^* |\Lambda(u)|}. \quad (\text{S24})$$

By substituting (S24) into (S23), we have  $m_{u,k(q)}^* = 0$ . Hence, conditions (S22c) and (S22d) are fulfilled. Note that as  $x_{i,k(q)}^t > 0$  in this case, the proof regarding the KKT conditions of  $x_{u,k(q)}$  can be achieved similarly. *Theorem 1* stands, and **Step 3** is implemented.  $\square$

#### D. Proof of Lemma 3

The difference between  $g(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'_{2(q)})$  and  $g(\psi'_{1(q)}, \psi'_{2(q)})$  in this case is also given by (S5). Considering the fact of  $a'_{u,k(q)}=0$  and,  $x'_{i,k(q)}>0$  the difference between  $g(\psi'_{1(q)}, \psi'_{2(q)})$  and  $g(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'_{2(q)})$  is:

$$g(\psi'_{1(q)}, \psi'_{2(q)}) - g(p'_{u,k(q)}, z'_{i,k(q)}, a'^{t-1}_{u,k(q)}, x'^{t-1}_{i,k(q)}, \psi'_{2(q)}) = -\frac{\lambda'_{(q)} |\Lambda(u)|}{2} (a'^{t-1}_{u,k(q)})^2 - \frac{\lambda'_{(q)} |\Lambda(i)|}{2} (x'^{t-1}_{i,k(q)} - x'^{t-1}_{i,k(q)})^2. \quad (\text{S25})$$

Moreover,  $g(\psi'_{1(q)}, \psi'_{2(q)})$  and  $g(\psi'_{1(q)}, \psi'^{t-1}_{2(q)})$  yields:

$$\begin{aligned} & g(\psi'_{1(q)}, \psi'_{2(q)}) - g(\psi'_{1(q)}, \psi'^{t-1}_{2(q)}) \\ &= (p'_{u,k(q)} - a'^{t-1}_{u,k(q)}) (h'_{u,k(q)} - h'^{t-1}_{u,k(q)}) + (z'_{i,k(q)} - x'^{t-1}_{i,k(q)}) (w'_{i,k(q)} - w'^{t-1}_{i,k(q)}) \\ &\stackrel{(I)}{=} \eta'_{(q)} \lambda'_{(q)} |\Lambda(u)| (p'_{u,k(q)} - a'^{t-1}_{u,k(q)})^2 + \frac{1}{\eta'_{(q)} \lambda'_{(q)} |\Lambda(i)|} (w'_{i,k(q)} - w'^{t-1}_{i,k(q)})^2 \\ &\stackrel{(II)}{\leq} \eta'_{(q)} \lambda'_{(q)} |\Lambda(u)| (p'_{u,k(q)})^2 + \frac{2|\Lambda(i)|}{\eta'_{(q)} \lambda'_{(q)}} \left( ((\eta'_{(q)} - 1) \lambda'_{(q)} z'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} z'^{t-1}_{i,k(q)})^2 + ((\eta'_{(q)} - 1) \lambda'_{(q)} x'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} x'^{t-1}_{i,k(q)})^2 \right), \end{aligned} \quad (\text{S26})$$

where (I) is based on the update rules of  $(h_{u,k(q)}, w_{i,k(q)})$  given in (4e), (4f) and (5c), and (II) is achieved with (22b) and  $a'_{u,k(q)}=0$ .

With (S5), (S25) and (S26), we have the following deduction:

$$\begin{aligned} & g(\psi'_{1(q)}, \psi'_{2(q)}) - g(\psi'^{t-1}_{1(q)}, \psi'^{t-1}_{2(q)}) \\ &\leq -\frac{1}{2} \left( \sum_{i \in \Lambda(u)} (z'^{t-1}_{i,k(q)})^2 + \lambda'_{(q)} |\Lambda(u)| \right) (p'_{u,k(q)} - p'^{t-1}_{u,k(q)})^2 - \frac{\lambda'_{(q)} |\Lambda(u)|}{2} (a'^{t-1}_{u,k(q)})^2 \\ &\quad - \frac{1}{2} \left( \sum_{u \in \Lambda(i)} (p'^{t-1}_{u,k(q)})^2 + \lambda'_{(q)} |\Lambda(i)| \right) (z'_{i,k(q)} - z'^{t-1}_{i,k(q)})^2 - \frac{\lambda'_{(q)} |\Lambda(i)|}{2} (x'_{i,k(q)} - x'^{t-1}_{i,k(q)})^2 \\ &\quad + \eta'_{(q)} \lambda'_{(q)} |\Lambda(u)| (p'_{u,k(q)})^2 + \frac{2|\Lambda(i)|}{\eta'_{(q)} \lambda'_{(q)}} \left( ((\eta'_{(q)} - 1) \lambda'_{(q)} z'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} z'^{t-1}_{i,k(q)})^2 + ((\eta'_{(q)} - 1) \lambda'_{(q)} x'_{i,k(q)} - (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} x'^{t-1}_{i,k(q)})^2 \right). \end{aligned} \quad (\text{S27})$$

Owing to (29), (25a) stands, which indicates that the augmented Lagrangian function (3) related to  $s_{(q)}$  or  $\tau_q$  is non-increasing as  $a'_{u,k(q)}=0$  and  $x'_{i,k(q)}>0$  in this case. Then after the  $t$ -th iteration, we substitute  $a'_{u,k(q)}=0$  into (S10):

$$\begin{aligned} g(\psi'_{1(q)}, \psi'_{2(q)}) &= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left( y_{u,i} - \sum_{l_1=1}^k p'_{u,l_1(q)} z'_{i,l_1(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right)^2 \\ &\quad + \sum_u |\Lambda(u)| \left( (\eta'_{(q)} - 1) \lambda'_{(q)} \left( \sum_{l_1=1}^{k-1} (p'_{u,l_1(q)} - a'^{t-1}_{u,l_1(q)})^2 + (p'_{u,k(q)})^2 \right) + (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} \sum_{l_2=k+1}^d (p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)})^2 \right) \\ &\quad + \sum_i |\Lambda(i)| \left( (\eta'_{(q)} - 1) \lambda'_{(q)} \sum_{l_1=1}^k (z'_{i,l_1(q)} - x'^{t-1}_{i,l_1(q)})^2 + (\eta'^{t-1}_{(q)} - 1) \lambda'^{t-1}_{(q)} \sum_{l_2=k+1}^d w'_{i,l_2(q)} (z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)})^2 \right) \\ &\quad + \sum_u \frac{\lambda'_{(q)} |\Lambda(u)|}{2} \left( \sum_{l_1=1}^{k-1} (p'_{u,l_1(q)} - a'^{t-1}_{u,l_1(q)})^2 + (p'_{u,k(q)})^2 + \sum_{l_2=k+1}^d (p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)})^2 \right) \\ &\quad + \sum_i \frac{\lambda'_{(q)} |\Lambda(i)|}{2} \left( \sum_{l_1=1}^k (z'_{i,l_1(q)} - x'^{t-1}_{i,l_1(q)})^2 + \sum_{l_2=k+1}^d (z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)})^2 \right). \end{aligned} \quad (\text{S28})$$

(S28) indicates that if (24b) is fulfilled, (25b) holds, thereby making (3) related to  $s_{(q)}$  or  $\tau_q$  lower-bounded as  $a'_{u,k(q)}=0$ , and  $x'_{i,k(q)}>0$  in this case. Based on the above inferences, *Lemma 2* stands, and **Step 4** is implemented.  $\square$

#### E. Proof of Theorem 2

**Part a.** Following Lemma 3,  $g(\psi_{1(q)}^t, \psi_{2(q)}^t)$  converges as  $t \rightarrow \infty$ , indicating that (S11) is fulfilled. With (26), (29) and (S27), we have (S12a), (S12b), (S12d), (S12f) and the following inferences:

$$\lim_{t \rightarrow \infty} a_{u,k(q)}^{t-1} \rightarrow 0, \quad (\text{S29a})$$

$$\lim_{t \rightarrow \infty} p_{u,k(q)}^t \rightarrow 0. \quad (\text{S29b})$$

Then according to (S12f), (S13b) is fulfilled. Hence, based on (S13b), (S29b) and  $a'_{u,k(q)}=0$ , (27) is fulfilled.

**Part b.** Firstly, considering a limit point  $\{\psi_{1(q)}^*, \psi_{2(q)}^*\}$  of a sequence  $\{\psi_{1(q)}^t, \psi_{2(q)}^t\}$  generated by the update rules of  $\{\psi_{1(q)}, \psi_{2(q)}\}$  based on (4) and (5), according to (27) and (S15), (S16) holds when  $a'_{u,k(q)}=0$ , and  $x'_{i,k(q)}>0$  in this case. Then considering the KKT conditions related to  $a_{u,k(q)}$ , i.e., (S22).

According to (S17)-(S21) and with  $a'_{u,k(q)}=0$ , conditions (S22a)-(S22c) are naturally satisfied. Thus, we focus on analyzing condition (S22d). Since we have  $a'_{u,k(q)}=0$  in this case, the following inequality holds:

$$p_{u,k(q)}^* + \frac{h_{u,k(q)}^*}{\lambda_{(q)}^* |\Lambda(u)|} \leq 0. \quad (\text{S30})$$

Note that (S30) indicates that:

$$m_{u,k(q)}^* = -\lambda_{(q)}^* |\Lambda(u)| \left( p_{u,k(q)}^* + \frac{h_{u,k(q)}^*}{\lambda_{(q)}^* |\Lambda(u)|} \right) \geq 0. \quad (\text{S31})$$

Thus, condition (S22) are all fulfilled in this case. Note that as  $x'_{i,k(q)}>0$  in this case, the proof regarding the KKT conditions of  $x_{u,k(q)}$  can be achieved similarly. *Theorem 2* stands, and **Step 5** is implemented. ■

## II. ADDITIONAL FIGURES

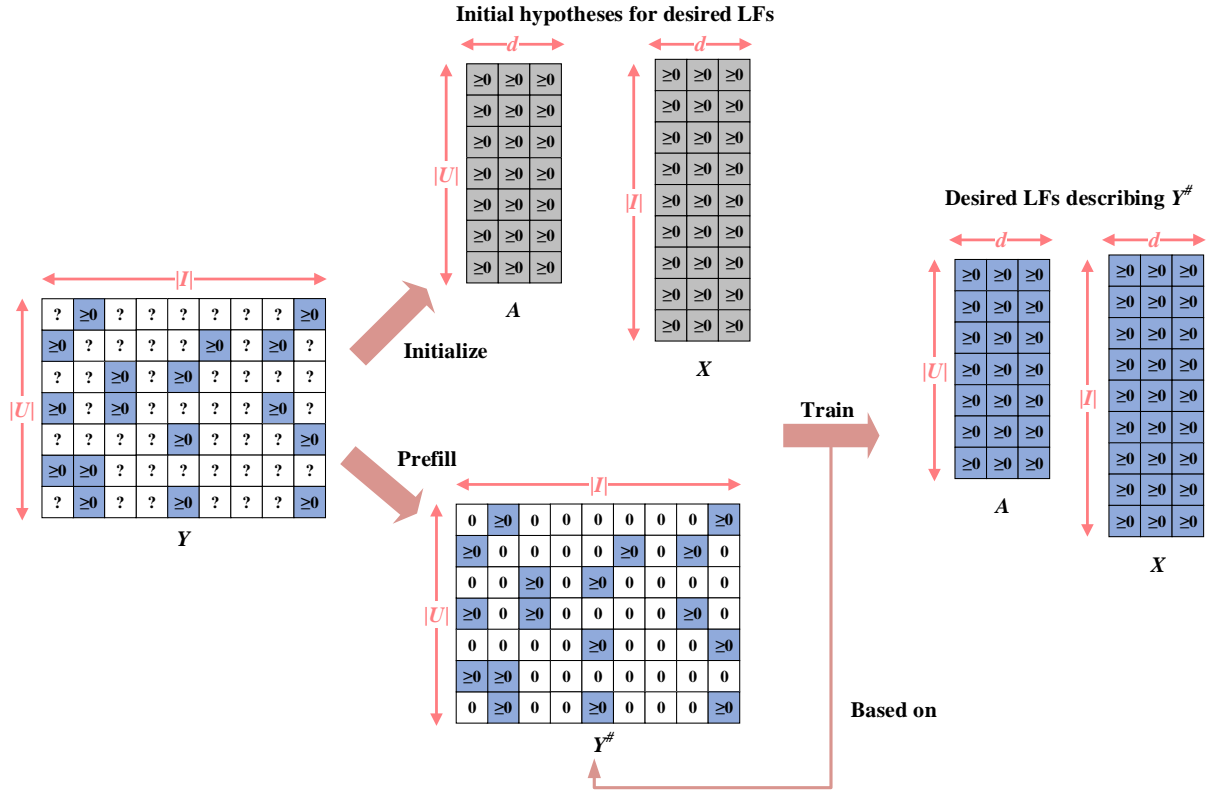


Fig. S1. Processing flow of an NMF model.

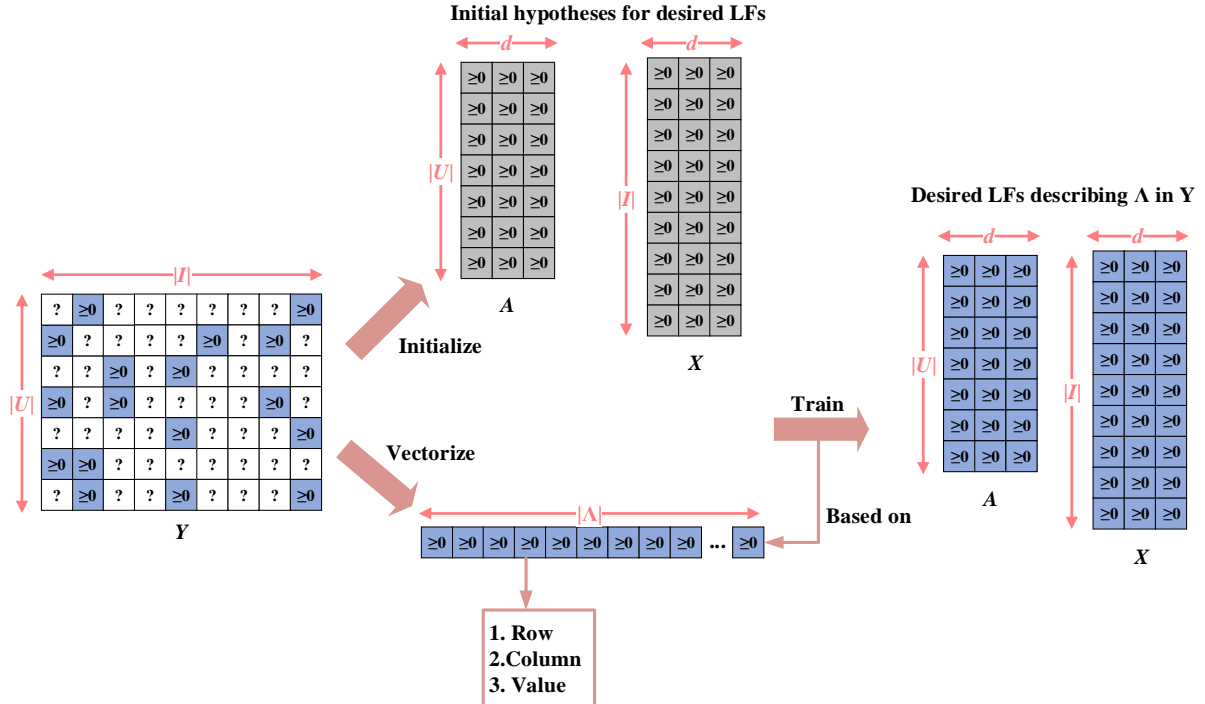


Fig. S2. Processing flow of an NLFA model.



## III. ADDITIONAL TABLES

TABLE S.I. Optimal Hyper-parameters during M1's ten times' training process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-2}, \eta=1$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-4}, \eta=2$	$\lambda=2^{-2}, \eta=1$	$\lambda=2^{-4}, \eta=2$
	MAE	$\lambda=2^{-2}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-2}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-2}, \eta=1$	$\lambda=2^{-4}, \eta=1$	$\lambda=2^{-4}, \eta=1$
D2	RMSE	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$
	MAE	$\lambda=1, \eta=2$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2$
D3	RMSE	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$
	MAE	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-2}$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-2}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2$
D4	RMSE	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$
	MAE	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2$	$\lambda=1, \eta=2$	$\lambda=1, \eta=1$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$	$\lambda=1, \eta=2^{-1}$

TABLE S.II. Optimal Hyper-parameters during M2's ten times' training process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\lambda=1.6$	$\lambda=1.6$	$\lambda=1.6$	$\lambda=1.8$	$\lambda=1.6$	$\lambda=1.8$	$\lambda=1.6$	$\lambda=1.8$	$\lambda=1.6$	$\lambda=1.6$
	MAE	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.2$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.2$
D2	RMSE	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$
	MAE	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$
D3	RMSE	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$
	MAE	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$	$\lambda=1.8$
D4	RMSE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure
	MAE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure

<sup>1</sup>M2 fails to obtain the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table VI.

TABLE S.III. Optimal Hyper-parameters during M3's ten times' training process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\mu=2^{-1}, p=1.9$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.7$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.7$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.9$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.8$
	MAE	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.9$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.7$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.7$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.9$	$\mu=2^{-1}, p=1.9$
D2	RMSE	$\mu=2, p=1.9$	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=2^{-1}, p=1.8$	$\mu=2^{-1}, p=1.9$	$\mu=2, p=1.9$	$\mu=2^{-1}, p=1.8$	$\mu=2, p=1.9$	$\mu=2, p=1.8$	$\mu=2, p=1.8$
	MAE	$\mu=4, p=1.9$	$\mu=2, p=1.9$	$\mu=2, p=1.8$	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=2, p=1.9$	$\mu=1, p=1.9$	$\mu=2, p=1.8$	$\mu=2, p=1.8$	$\mu=2, p=1.9$
D3	RMSE	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=2, p=1.8$	$\mu=2, p=1.8$	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=2, p=1.9$	$\mu=2, p=1.9$	$\mu=2, p=1.9$	$\mu=2, p=1.9$
	MAE	$\mu=2, p=1.9$	$\mu=2, p=1.8$	$\mu=2, p=1.9$	$\mu=2, p=1.8$	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=4, p=1.9$	$\mu=2, p=1.8$	$\mu=2, p=1.9$	$\mu=2, p=1.9$
D4	RMSE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure
	MAE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure

<sup>1</sup>M3 fails to obtain the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table VI.

TABLE S.IV. Optimal Hyper-parameters during M4's ten times' training process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$
	MAE	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$
D2	RMSE	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^2$	$\alpha=10^3, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^3$	$\alpha=10^4, \beta=10^2$	$\alpha=10^3, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^2$	$\alpha=10^3, \beta=10^3$
	MAE	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^3$
D3	RMSE	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$
	MAE	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^3, \beta=10^4$	$\alpha=10^4, \beta=10^3$	$\alpha=10^3, \beta=10^4$
D4	RMSE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure
	MAE	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure

<sup>1</sup>M4 fails to obtain the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table VI.



TABLE S.VIII. RMSE, MAE and Time Cost of M1, M8 and M9 on D1-4.

Dataset	Model	Case	Prediction Accuracy	<sup>1</sup> Tuning Time Cost (Secs)	<sup>2</sup> Testing Time Cost (Secs)	Total Time Cost (Secs)
D1	M1	RMSE	0.2373 $\pm 2.2\text{E-}6$	428 $\pm 22.7$	6 $\pm 2.4$	434 $\pm 25$
		MAE	0.1815 $\pm 1.1\text{E-}6$	439 $\pm 25.4$	6 $\pm 2.8$	445 $\pm 28$
	M8	RMSE	<b>0.2339 <math>\pm 2.7\text{E-}4</math></b>	-	-	<b>46 <math>\pm 4</math></b>
		MAE	<b>0.1793 <math>\pm 3.3\text{E-}4</math></b>	-	-	<b>60 <math>\pm 5</math></b>
	M9	RMSE	0.2573 $\pm 1.4\text{E-}6$	-	-	387 $\pm 33$
		MAE	0.2015 $\pm 2.8\text{E-}6$	-	-	396 $\pm 46$
D2	M1	RMSE	1.0187 $\pm 1.1\text{E-}6$	271 $\pm 45.4$	4 $\pm 1.7$	275 $\pm 47$
		MAE	0.8079 $\pm 2.5\text{E-}6$	305 $\pm 38.3$	3 $\pm 0.9$	308 $\pm 39$
	M8	RMSE	<b>1.0158 <math>\pm 6.4\text{E-}4</math></b>	-	-	<b>25 <math>\pm 5</math></b>
		MAE	<b>0.7848 <math>\pm 9.3\text{E-}4</math></b>	-	-	<b>29 <math>\pm 8</math></b>
	M9	RMSE	1.0209 $\pm 2.0\text{E-}5$	-	-	87 $\pm 11$
		MAE	0.7883 $\pm 1.3\text{E-}5$	-	-	85 $\pm 9$
D3	M1	RMSE	<b>0.8665 <math>\pm 7.8\text{E-}4</math></b>	739 $\pm 72.3$	21 $\pm 14.7$	759 $\pm 87$
		MAE	0.6829 $\pm 1.7\text{E-}6$	756 $\pm 53.8$	3 $\pm 0.5$	763 $\pm 54$
	M8	RMSE	0.8673 $\pm 1.3\text{E-}3$	-	-	<b>26 <math>\pm 6</math></b>
		MAE	<b>0.6785 <math>\pm 9.6\text{E-}5</math></b>	-	-	<b>30 <math>\pm 9</math></b>
	M9	RMSE	0.8684 $\pm 4.7\text{E-}4$	-	-	487 $\pm 59$
		MAE	0.6793 $\pm 2.8\text{E-}5$	-	-	268 $\pm 40$
D4	M1	RMSE	0.8096 $\pm 2.9\text{E-}6$	2,934 $\pm 353.8$	38 $\pm 24.6$	3,972 $\pm 378$
		MAE	0.6221 $\pm 7.9\text{E-}7$	9,203 $\pm 828.9$	33 $\pm 20.4$	9,236 $\pm 849$
	M8	RMSE	0.8091 $\pm 3.0\text{E-}3$	-	-	<b>334 <math>\pm 46</math></b>
		MAE	<b>0.6191 <math>\pm 1.7\text{E-}4</math></b>	-	-	<b>358 <math>\pm 31</math></b>
	M9	RMSE	<b>0.8086 <math>\pm 6.0\text{E-}5</math></b>	-	-	3731 $\pm 311$
		MAE	0.6199 $\pm 7.1\text{E-}6$	-	-	5532 $\pm 566$

<sup>1</sup>Time cost consumed by M1 for manually grid-searching optimal hyper-parameters; <sup>2</sup>Time cost consumed by M1 with obtained hyper-parameters.

TABLE S.IX. RMSE/MAE of M1-9 on D1-4, including Win/Loss counts and Friedman Rank, where ● indicates that both M8 and M9 have higher RMSE/MAE than the rival models

No.	Case	M1	M2	M3	M4	M5	M6	M7	M8	M9
D1	RMSE	0.2373 $\pm 2.2\text{E-}6$	0.3058 $\pm 5.0\text{E-}4$	0.3047 $\pm 4.3\text{E-}5$	0.2384 $\pm 1.0\text{E-}4$	0.4913 $\pm 1.0\text{E-}4$	●0.2302 $\pm 2.6\text{E-}3$	0.2504 $\pm 4.7\text{E-}4$	0.2339 $\pm 2.7\text{E-}4$	0.2573 $\pm 1.4\text{E-}6$
	MAE	0.1815 $\pm 1.1\text{E-}6$	0.2439 $\pm 4.4\text{E-}5$	0.2422 $\pm 3.2\text{E-}5$	0.1832 $\pm 4.8\text{E-}5$	0.4111 $\pm 1.6\text{E-}2$	●0.1792 $\pm 7.9\text{E-}5$	0.1953 $\pm 8.9\text{E-}4$	0.1793 $\pm 3.3\text{E-}4$	0.2015 $\pm 2.8\text{E-}6$
D2	RMSE	1.0187 $\pm 1.1\text{E-}6$	1.1281 $\pm 7.2\text{E-}3$	1.1257 $\pm 1.8\text{E-}4$	1.0787 $\pm 8.6\text{E-}7$	1.8808 $\pm 2.8\text{E-}2$	1.1494 $\pm 4.1\text{E-}5$	1.0255 $\pm 4.5\text{E-}4$	<b>1.0158 <math>\pm 6.4\text{E-}4</math></b>	1.0209 $\pm 2.0\text{E-}5$
	MAE	0.8079 $\pm 2.5\text{E-}6$	0.9256 $\pm 1.5\text{E-}3$	0.9229 $\pm 1.9\text{E-}4$	0.8580 $\pm 6.2\text{E-}6$	1.5403 $\pm 2.6\text{E-}2$	0.9257 $\pm 2.1\text{E-}4$	0.7945 $\pm 1.6\text{E-}3$	<b>0.7848 <math>\pm 9.3\text{E-}4</math></b>	0.7883 $\pm 1.3\text{E-}5$
D3	RMSE	●0.8665 $\pm 7.8\text{E-}4$	1.0336 $\pm 5.4\text{E-}4$	1.0848 $\pm 5.3\text{E-}5$	0.8713 $\pm 3.7\text{E-}4$	2.2963 $\pm 9.8\text{E-}3$	0.8845 $\pm 1.1\text{E-}3$	0.8972 $\pm 8.2\text{E-}3$	0.8673 $\pm 1.3\text{E-}3$	0.8684 $\pm 4.7\text{E-}4$
	MAE	0.6829 $\pm 1.7\text{E-}6$	0.8832 $\pm 4.0\text{E-}4$	0.9021 $\pm 4.2\text{E-}5$	0.6802 $\pm 3.3\text{E-}4$	1.9190 $\pm 9.6\text{E-}3$	0.7021 $\pm 5.5\text{E-}3$	0.7036 $\pm 3.6\text{E-}3$	<b>0.6785 <math>\pm 9.6\text{E-}5</math></b>	0.6793 $\pm 2.8\text{E-}5$
D4	RMSE	0.8096 $\pm 2.9\text{E-}6$	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	0.8436 $\pm 1.2\text{E-}3$	0.8574 $\pm 1.2\text{E-}3$	0.8091 $\pm 3.0\text{E-}3$	<b>0.8086 <math>\pm 6.0\text{E-}5</math></b>
	MAE	0.6221 $\pm 7.9\text{E-}7$	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	0.6530 $\pm 4.9\text{E-}3$	0.6647 $\pm 3.3\text{E-}3$	<b>0.6191 <math>\pm 1.7\text{E-}4</math></b>	0.6199 $\pm 7.1\text{E-}6$
Win/Loss		8/1	9/0	9/0	9/0	9/0	7/2	9/0	-	-
F-Rank		2.875	7.375	7.125	5	8.625	4.5	4.875	<b>1.5</b>	3.125

<sup>1</sup>M2-M5 fails to obtain the final results on D4 on our experimental environment as shown in Table VI.

TABLE S.X. Total time cost of M1-9 in RMSE/MAE on D1-4 (Secs), including Win/Loss counts and Friedman Rank

No.	Case	M1	M2	M3	M4	M5	M6	M7	M8	M9
D1	RMSE	434 $\pm 25$	38,499 $\pm 2,332$	43,271 $\pm 2,962$	209,670 $\pm 36,625$	3,856 $\pm 578$	10,804 $\pm 832$	2,011,581 $\pm 481,806$	<b>46 <math>\pm 4</math></b>	387 $\pm 33$
	MAE	445 $\pm 28$	51,443 $\pm 2,643$	189,090 $\pm 29,135$	210,745 $\pm 27,190$	3,912 $\pm 103$	13,432 $\pm 2,219$	1,809,472 $\pm 393,344$	<b>60 <math>\pm 5</math></b>	396 $\pm 46$
D2	RMSE	275 $\pm 47$	236 $\pm 35$	128 $\pm 21$	138 $\pm 39$	55 $\pm 7$	2,109 $\pm 295$	888,704 $\pm 223,355$	<b>25 <math>\pm 5</math></b>	87 $\pm 11$
	MAE	308 $\pm 39$	32 $\pm 3$	128 $\pm 27$	766 $\pm 64$	56 $\pm 6$	2,256 $\pm 333$	2,015,970 $\pm 861,492$	<b>29 <math>\pm 8</math></b>	85 $\pm 9$
D3	RMSE	759 $\pm 87$	42,578 $\pm 3,258$	71,927 $\pm 2,718$	45,849 $\pm 2,479$	717 $\pm 22$	8,359 $\pm 532$	883,008 $\pm 63,588$	<b>26 <math>\pm 6</math></b>	487 $\pm 59$
	MAE	763 $\pm 54$	1,906 $\pm 291$	12,294 $\pm 2,478$	48,821 $\pm 2,363$	716 $\pm 53$	7,700 $\pm 219$	676,921 $\pm 41,748$	<b>30 <math>\pm 9</math></b>	268 $\pm 40$
D4	RMSE	3,972 $\pm 378$	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	266,885 $\pm 12,775$	45,533,828 $\pm 8,105,384$	<b>334 <math>\pm 46</math></b>	3731 $\pm 311$
	MAE	9,236 $\pm 849$	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	<sup>1</sup> Failure	232,974 $\pm 13,157$	50,643,155 $\pm 6,301,613$	<b>358 <math>\pm 31</math></b>	5532 $\pm 566$
Win/Loss		9/0	9/0	9/0	9/0	9/0	9/0	9/0	-	-
F-Rank		4.125	5.75	6.625	7.25	4.25	5.625	8	<b>1</b>	2.375

<sup>1</sup>M2-M5 fails to obtain the final results on D4 on our experimental environment as shown in Table VI.