

An Adaptive Alternating-direction-method of Multipliers-Incorporated Approach to Nonnegative Latent Factor Analysis: Supplementary File

This is the supplementary file for the paper entitled *An Adaptive Alternating-direction-method of Multipliers-incorporated Approach to Non-negative Latent Factor Analysis*. Detailed convergence proof of A²NLF, additional experimental results and several supplementary files are presented here.

I. CONVERGENCE OF A²NLF

A. Proof of Lemma 1

Note that A²NLF's learning objective is non-convex. 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 (17) 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 (18) holds based on (S3). Hence, Lemma 1 holds, and **Step 1** is implemented. \square

B. Proof of Lemma 2

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

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

Considering (5a)'s optimality condition, (S4) is transformed as:

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

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

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

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

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

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:

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

Owing to (20a), (21a) stands, which indicates that the augmented Lagrangian function (3) related to the q -th particle is non-increasing as $a'^t_{u,k(q)} > 0$ and $x'^t_{i,k(q)} > 0$. Then after the t -th iteration, the partial objective from (3) related to the q -th particle is formulated as:

$$\begin{aligned}
& g\left(s'^t_{1(q)}, s'^t_{2(q)}\right) \\
&= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left(y_{u,i} - \sum_{l_1=1}^k p'^t_{u,l_1(q)} z'^t_{i,l_1(q)} - \sum_{l_2=k+1}^d p'^{t-1}_{u,l_2(q)} z'^{t-1}_{i,l_2(q)} \right)^2 \\
&+ \sum_u \left(\left(\sum_{l_1=1}^k h'^t_{u,l_1(q)} \left(p'^t_{u,l_1(q)} - a'^t_{u,l_1(q)} \right) \right) + \left(\sum_{l_2=k+1}^d h'^{t-1}_{u,l_2(q)} \left(p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)} \right) \right) \right) + \sum_i \left(\left(\sum_{l_1=1}^k w'^t_{i,l_1(q)} \left(z'^t_{i,l_1(q)} - x'^t_{i,l_1(q)} \right) \right) + \left(\sum_{l_2=k+1}^d w'^{t-1}_{i,l_2(q)} \left(z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)} \right) \right) \right) \\
&+ \sum_u \frac{\lambda'_{(q)} |\Lambda(u)|}{2} \left(\sum_{l_1=1}^k \left(p'^t_{u,l_1(q)} - a'^t_{u,l_1(q)} \right)^2 + \sum_{l_2=k+1}^d \left(p'^{t-1}_{u,l_2(q)} - a'^{t-1}_{u,l_2(q)} \right)^2 \right) + \sum_i \frac{\lambda'_{(q)} |\Lambda(i)|}{2} \left(\sum_{l_1=1}^k \left(z'^t_{i,l_1(q)} - x'^t_{i,l_1(q)} \right)^2 + \sum_{l_2=k+1}^d \left(z'^{t-1}_{i,l_2(q)} - x'^{t-1}_{i,l_2(q)} \right)^2 \right).
\end{aligned} \tag{S9}$$

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

$$\begin{aligned}
& g(s_{1(q)}^t, s_{2(q)}^t) \\
&= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left(y_{u,i} - \sum_{l_1=1}^k p_{u,l_1}^t z_{i,l_1(q)}^t - \sum_{l_2=k+1}^d p_{u,l_2}^{t-1} z_{i,l_2(q)}^{t-1} \right)^2 \\
&+ \sum_u |\Lambda(u)| \left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t \sum_{l_1=1}^k \left(p_{u,l_1}^t - a_{u,l_1}^t \right)^2 + \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} \sum_{l_2=k+1}^d \left(p_{u,l_2}^{t-1} - a_{u,l_2}^{t-1} \right)^2 \right) \\
&+ \sum_i |\Lambda(i)| \left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t \sum_{l_1=1}^k \left(z_{i,l_1}^t - x_{i,l_1}^t \right)^2 + \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} \sum_{l_2=k+1}^d w_{i,l_2}^t \left(z_{i,l_2}^{t-1} - x_{i,l_2}^{t-1} \right)^2 \right) \\
&+ \sum_u \frac{\lambda_{(q)}^t |\Lambda(u)|}{2} \left(\sum_{l_1=1}^k \left(p_{u,l_1}^t - a_{u,l_1}^t \right)^2 + \sum_{l_2=k+1}^d \left(p_{u,l_2}^{t-1} - a_{u,l_2}^{t-1} \right)^2 \right) + \sum_i \frac{\lambda_{(q)}^t |\Lambda(i)|}{2} \left(\sum_{l_1=1}^k \left(z_{i,l_1}^t - x_{i,l_1}^t \right)^2 + \sum_{l_2=k+1}^d \left(z_{i,l_2}^{t-1} - x_{i,l_2}^{t-1} \right)^2 \right).
\end{aligned} \tag{S10}$$

(S10) indicates that if (20b) is fulfilled, (21b) holds, thereby making (3) related to the q -th particle lower-bounded as $a_{u,k(q)}^t > 0$ and $x_{i,k(q)}^t > 0$. Based on the above inferences, *Lemma 2* stands, and **Step 2** is implemented. \square

C. Proof of Theorem 1

Part a. Following *Lemma 2*, $g(s_{1(q)}^t, s_{2(q)}^t)$ converges as $t \rightarrow \infty$, indicating that:

$$\lim_{t \rightarrow \infty} g(s_{1(q)}^t, s_{2(q)}^t) - g(s_{1(q)}^{t-1}, s_{2(q)}^{t-1}) \rightarrow 0. \tag{S11}$$

With (20), when (S1) is fulfilled, the upper-bound of $g(s_{1(q)}^t, s_{2(q)}^t) - g(s_{1(q)}^{t-1}, s_{2(q)}^{t-1})$ is zero as $t \rightarrow \infty$, thereby achieving (22). Following (S8) and (22), we have [1]:

$$\lim_{t \rightarrow \infty} (p_{u,k(q)}^t - p_{u,k(q)}^{t-1}) \rightarrow 0, \tag{S12a}$$

$$\lim_{t \rightarrow \infty} (z_{i,k(q)}^t - z_{i,k(q)}^{t-1}) \rightarrow 0, \tag{S12b}$$

$$\lim_{t \rightarrow \infty} (a_{u,k(q)}^t - a_{u,k(q)}^{t-1}) \rightarrow 0, \tag{S12c}$$

$$\lim_{t \rightarrow \infty} (x_{i,k(q)}^t - x_{i,k(q)}^{t-1}) \rightarrow 0, \tag{S12d}$$

$$\lim_{t \rightarrow \infty} \left(\left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t p_{u,k(q)}^t - \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} p_{u,k(q)}^{t-1} \right)^2 + \left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t a_{u,k(q)}^t - \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} a_{u,k(q)}^{t-1} \right)^2 \right) \rightarrow 0, \tag{S12e}$$

$$\lim_{t \rightarrow \infty} \left(\left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t z_{i,k(q)}^t - \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} z_{i,k(q)}^{t-1} \right)^2 + \left(\left(\eta_{(q)}^t - 1 \right) \lambda_{(q)}^t x_{i,k(q)}^t - \left(\eta_{(q)}^{t-1} - 1 \right) \lambda_{(q)}^{t-1} x_{i,k(q)}^{t-1} \right)^2 \right) \rightarrow 0. \tag{S12f}$$

Based on (17), (18) and (S12), we have the following inferences:

$$\lim_{t \rightarrow \infty} (h_{u,k(q)}^t - h_{u,k(q)}^{t-1}) \rightarrow 0, \tag{S13a}$$

$$\lim_{t \rightarrow \infty} (w_{i,k(q)}^t - w_{i,k(q)}^{t-1}) \rightarrow 0. \tag{S13b}$$

Based on (4e), (4f) and (S13), we conclude that (23) 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 (23) 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 $\{s_{1(q)}^*, s_{2(q)}^*\}$ of a sequence $\{s_{1(q)}^t, s_{2(q)}^t\}$ generated by the update rules of $\{s_{1(q)}, s_{2(q)}\}$ based on (4)

and (5), the following KKT conditions are satisfied with (23) 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) [1, 21]:

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

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 an A²NLF model's learning rules 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 $g(p_{u,k(q)}^t, z_{i,k(q)}^t, a_{u,k(q)}^{t-1}, x_{i,k(q)}^{t-1}, s_{2(q)}^{t-1})$ and $g(s_{1(q)}^{t-1}, s_{2(q)}^{t-1})$ in this case is also given by (S5). Considering the fact of $a_{u,k(q)}^t=0$ and, $x_{i,k(q)}^t>0$ the difference between $g(s_{1(q)}^t, s_{2(q)}^{t-1})$ and $g(p_{u,k(q)}^t, z_{i,k(q)}^t, a_{u,k(q)}^{t-1}, x_{i,k(q)}^{t-1}, s_{2(q)}^{t-1})$ is:

$$g(s_{1(q)}^t, s_{2(q)}^{t-1}) - g(p_{u,k(q)}^t, z_{i,k(q)}^t, a_{u,k(q)}^{t-1}, x_{i,k(q)}^{t-1}, s_{2(q)}^{t-1}) = -\frac{\lambda_{(q)}^t |\Lambda(u)|}{2} (a_{u,k(q)}^{t-1})^2 - \frac{\lambda_{(q)}^t |\Lambda(i)|}{2} (x_{i,k(q)}^t - x_{i,k(q)}^{t-1})^2. \quad (\text{S25})$$

Moreover, $g(s_{1(q)}^t, s_{2(q)}^t)$ and $g(s_{1(q)}^t, s_{2(q)}^{t-1})$ yields:

$$\begin{aligned} & g(s_{1(q)}^t, s_{2(q)}^t) - g(s_{1(q)}^t, s_{2(q)}^{t-1}) \\ &= (p_{u,k(q)}^t - a_{u,k(q)}^t)(h_{u,k(q)}^t - h_{u,k(q)}^{t-1}) + (z_{i,k(q)}^t - x_{i,k(q)}^{t-1})(w_{i,k(q)}^t - w_{i,k(q)}^{t-1}) \\ &\stackrel{(I)}{=} \eta_{(q)}^t \lambda_{(q)}^t |\Lambda(u)| (p_{u,k(q)}^t - a_{u,k(q)}^t)^2 + \frac{1}{\eta_{(q)}^t \lambda_{(q)}^t |\Lambda(i)|} (w_{i,k(q)}^t - w_{i,k(q)}^{t-1})^2 \\ &\stackrel{(II)}{\leq} \eta_{(q)}^t \lambda_{(q)}^t |\Lambda(u)| (p_{u,k(q)}^t)^2 + \frac{2|\Lambda(i)|}{\eta_{(q)}^t \lambda_{(q)}^t} \left(((\eta_{(q)}^t - 1) \lambda_{(q)}^t z_{i,k(q)}^t - (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} z_{i,k(q)}^{t-1})^2 + ((\eta_{(q)}^t - 1) \lambda_{(q)}^t x_{i,k(q)}^t - (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} x_{i,k(q)}^{t-1})^2 \right), \end{aligned} \quad (\text{S26})$$

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 (18) and $a_{u,k(q)}^t=0$.

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

$$\begin{aligned} & g(s_{1(q)}^t, s_{2(q)}^t) - g(s_{1(q)}^{t-1}, s_{2(q)}^{t-1}) \\ &\leq -\frac{1}{2} \left(\sum_{i \in \Lambda(u)} (z_{i,k(q)}^{t-1})^2 + \lambda_{(q)}^t |\Lambda(u)| \right) (p_{u,k(q)}^t - p_{u,k(q)}^{t-1})^2 - \frac{\lambda_{(q)}^t |\Lambda(u)|}{2} (a_{u,k(q)}^{t-1})^2 \\ &\quad - \frac{1}{2} \left(\sum_{u \in \Lambda(i)} (p_{u,k(q)}^{t-1})^2 + \lambda_{(q)}^t |\Lambda(i)| \right) (z_{i,k(q)}^t - z_{i,k(q)}^{t-1})^2 - \frac{\lambda_{(q)}^t |\Lambda(i)|}{2} (x_{i,k(q)}^t - x_{i,k(q)}^{t-1})^2 \\ &\quad + \eta_{(q)}^t \lambda_{(q)}^t |\Lambda(u)| (p_{u,k(q)}^t)^2 + \frac{2|\Lambda(i)|}{\eta_{(q)}^t \lambda_{(q)}^t} \left(((\eta_{(q)}^t - 1) \lambda_{(q)}^t z_{i,k(q)}^t - (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} z_{i,k(q)}^{t-1})^2 + ((\eta_{(q)}^t - 1) \lambda_{(q)}^t x_{i,k(q)}^t - (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} x_{i,k(q)}^{t-1})^2 \right). \end{aligned} \quad (\text{S27})$$

Owing to (25), (21a) stands, which indicates that the augmented Lagrangian function (3) related to the q -th particle is non-increasing as $a_{u,k(q)}^t=0$ and $x_{i,k(q)}^t>0$ in this case. Then after the t -th iteration, we substitute $a_{u,k(q)}^t=0$ into (S10):

$$\begin{aligned} g(s_{1(q)}^t, s_{2(q)}^t) &= \frac{1}{2} \sum_{y_{u,i} \in \Lambda} \left(y_{u,i} - \sum_{l_1=1}^k p_{u,l_1(q)}^t z_{i,l_1(q)}^t - \sum_{l_2=k+1}^d p_{u,l_2(q)}^{t-1} z_{i,l_2(q)}^{t-1} \right)^2 \\ &\quad + \sum_u |\Lambda(u)| \left((\eta_{(q)}^t - 1) \lambda_{(q)}^t \left(\sum_{l_1=1}^{k-1} (p_{u,l_1(q)}^t - a_{u,l_1(q)}^t)^2 + (p_{u,k(q)}^t)^2 \right) + (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} \sum_{l_2=k+1}^d (p_{u,l_2(q)}^{t-1} - a_{u,l_2(q)}^{t-1})^2 \right) \\ &\quad + \sum_i |\Lambda(i)| \left((\eta_{(q)}^t - 1) \lambda_{(q)}^t \sum_{l_1=1}^k (z_{i,l_1(q)}^t - x_{i,l_1(q)}^{t-1})^2 + (\eta_{(q)}^{t-1} - 1) \lambda_{(q)}^{t-1} \sum_{l_2=k+1}^d w_{i,l_2(q)}^t (z_{i,l_2(q)}^{t-1} - x_{i,l_2(q)}^{t-1})^2 \right) \\ &\quad + \sum_u \frac{\lambda_{(q)}^t |\Lambda(u)|}{2} \left(\sum_{l_1=1}^{k-1} (p_{u,l_1(q)}^t - a_{u,l_1(q)}^t)^2 + (p_{u,k(q)}^t)^2 + \sum_{l_2=k+1}^d (p_{u,l_2(q)}^{t-1} - a_{u,l_2(q)}^{t-1})^2 \right) \\ &\quad + \sum_i \frac{\lambda_{(q)}^t |\Lambda(i)|}{2} \left(\sum_{l_1=1}^k (z_{i,l_1(q)}^t - x_{i,l_1(q)}^{t-1})^2 + \sum_{l_2=k+1}^d (z_{i,l_2(q)}^{t-1} - x_{i,l_2(q)}^{t-1})^2 \right). \end{aligned} \quad (\text{S28})$$

(S28) indicates that if (20b) is fulfilled, (21b) holds, thereby making (3) related to the q -th particle lower-bounded as $a_{u,k(q)}^t=0$, and $x_{i,k(q)}^t>0$ 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*, $g(s_{1(q)}^t, s_{2(q)}^t)$ converges as $t \rightarrow \infty$, indicating that (S11) is fulfilled. With (22), (25) 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 $a'_{u,k(q)}=0$, (23) is fulfilled.

Part b. Firstly, considering a limit point $\{s_{1(q)}^*, s_{2(q)}^*\}$ of a sequence $\{s_{1(q)}^t, s_{2(q)}^t\}$ generated by the update rules of $\{s_{1(q)}, s_{2(q)}\}$ based on (4) and (5), according to (23) 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. SUPPLEMENTARY TABLES

TABLE S1. PSO Parameters Settings in (7).

w	c_1	c_2	r_1, r_2
0.729	2	2	uniform random numbers $\in [0,1]$.

TABLE S2 PSO PARAMETERS SETTINGS IN (13)

$\tilde{\lambda}$	$\hat{\lambda}$	$\tilde{\eta}$	$\hat{\eta}$	\tilde{v}_{λ}	\hat{v}_{λ}	\tilde{v}_{η}	\hat{v}_{η}
0.2	2	1	2	$-\hat{v}_{\lambda}$	$0.2 \times (\hat{\lambda} - \tilde{\lambda})$	$-\hat{v}_{\eta}$	$0.2 \times (\hat{\eta} - \tilde{\eta})$

TABLE S3. Grid-search Range of Hyper-parameters in M1-6 on D1-4.

No.	Hyper-parameters	Grid-searching Range
M1	Augmentation coefficient λ	$2^{-6}, 2^{-4}, 2^{-2}, 1, 2^2, 2^4, 2^6, 2^8$
	Learning rate η	$8, 4, 2, 1, 2^{-1}, 2^{-2}, 2^{-3}$
M2	Penalty coefficient λ	$2, 1.8, 1.6, 1.4, 1.2, 1.0, 0.8$
M3	Regularization coefficient μ	$8, 4, 2, 1, 2^{-1}, 2^{-2}, 2^{-3}$
	L_p coefficient p	$1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0$
M4	Penalty coefficient α	$1, 10, 10^2, 10^3, 10^4, 10^5$
	Penalty coefficient β	$10, 10^2, 10^3, 10^4, 10^5, 10^6$
M5	Penalty coefficient ρ	$2^{-3}, 2^{-5}, 2^{-7}, 2^{-9}, 2^{-11}, 2^{-13}, 2^{-15}, 2^{-17}$
	Regularization coefficient λ	$10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 0.1, 1$
M6	Learning rate η	$10^{-5}, 5 \times 10^{-5}, 10^{-4}, 5 \times 10^{-4}, 10^{-3}, 5 \times 10^{-3}, 10^{-2}$
	Batch size bs	$32, 64, 128, 256, 512, 1024$
	Regularization coefficient λ	$10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 0.1, 1$
M7	Learning rate η	$10^{-5}, 5 \times 10^{-5}, 10^{-4}, 5 \times 10^{-4}, 10^{-3}, 5 \times 10^{-3}, 10^{-2}$
	Batch size bs	$32, 64, 128, 256, 512, 1024$

TABLE S4. 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 S5. 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	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure
	MAE	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure

¹Note that M2 fails to achieve the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table V.

TABLE S6. 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	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure
	MAE	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure

¹Note that M3 fails to achieve the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table V.

TABLE S7. 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	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure
	MAE	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure	¹ Failure

¹Note that M4 fails to achieve the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table V.

TABLE S8. Optimal Hyper-parameters during M5’s ten times’ training process on D1-4

[illegible]

¹Note that M5 fails to achieve the final results on D4: their memory requirements are too large to meet on our experimental environment as shown in Table V.

TABLE S9. Optimal Hyper-parameters during M6’s ten times’ training process on D1-4

[illegible]

¹Note that bs denotes batch size adopted by M6 on an HDI matrix;

TABLE S10. Optimal Hyper-parameters during M7’s ten times’ training process on D1-4

[illegible]

TABLE S11. RMSE and Time Cost of M1 and M8 on D1-4.

Dataset	Model	Prediction Accuracy	¹ Tuning Time Cost (Secs)	² Testing Time Cost (Secs)	Total Time Cost (Secs)
D1	M1	RMSE	0.2373 \pm 2.2E-6	428 \pm 22.7	434 \pm 25
		MAE	0.1815 \pm 1.1E-6	439 \pm 25.4	445 \pm 28
	M8	RMSE	0.2339 \pm 2.7E-4	-	46 \pm 4
		MAE	0.1792 \pm 3.3E-4	-	60 \pm 5
D2	M1	RMSE	1.0187 \pm 1.1E-6	271 \pm 45.4	275 \pm 47
		MAE	0.8079 \pm 2.5E-6	305 \pm 38.3	308 \pm 39
	M8	RMSE	1.0172 \pm 7.4E-4	-	25 \pm 5
		MAE	0.7856 \pm 7.9E-4	-	29 \pm 8
D3	M1	RMSE	0.8665 \pm 7.8E-4	739 \pm 72.3	759 \pm 87
		MAE	0.6829 \pm 1.7E-6	756 \pm 53.8	763 \pm 54
	M8	RMSE	0.8675 \pm 8.2E-4	-	26 \pm 6
		MAE	0.6787 \pm 7.3E-4	-	30 \pm 9
D4	M1	RMSE	0.8096 \pm 2.9E-6	2,934 \pm 353.8	2,972 \pm 378
		MAE	0.6221 \pm 7.9E-7	9,203 \pm 828.9	9,236 \pm 849
	M8	RMSE	0.8089 \pm 9.4E-4	-	334 \pm 46
		MAE	0.6193 \pm 5.1E-4	-	358 \pm 31

¹Time cost consumed by M1 for manually grid-searching optimal hyper-parameters; ²Time cost consumed by M1 with achieved hyper-parameters.

TABLE S12. Storage Complexity and Memory Requirements of M1-8 on D1-4.

No.	Storage Complexity	Memory Requirements (GB)			
		D1	D2	D3	D4
M1	$\Theta((U + I) \times d + \Lambda)$	0.7	0.6	0.5	1.7
M2	$\Theta(U \times I)$	17.6	1.8	9.3	>256
M3	$\Theta(U \times I)$	15.4	1.9	8.6	>256
M4	$\Theta(U \times I)$	21.9	3.5	11.5	>256
M5	$\Theta(U \times I)$	26.5	3.9	12.7	>256
M6	$\Theta(^1bs \times U + \Lambda)$	2.9	1.7	1.7	3.1
M7	$\Theta((U + I) \times d + bs \times ^21^stLN + \Lambda)$	2.1	1.2	1.8	6.5
M8	$\Theta((U + I) \times d + \Lambda)$	0.7	0.6	0.5	1.7

¹bs denotes batch size adopted by M6 and M7 on an HDI matrix; ²1stLN denotes the number of neuron in the 1st layer and is set at $2 \times d$ according to [10].

TABLE S13. RMSE/MAE of M1-8 on D1-4, including Win/Loss counts and Friedman Rank, where ● indicates that M8 has higher RMSE/MAE than the rival models

No.	CASE	M1	M2	M3	M4	M5	M6	M7	M8
D1	RMSE	0.2373 \pm 2.2E-6	0.3058 \pm 5.0E-4	0.3047 \pm 4.3E-5	0.2384 \pm 1.0E-4	0.4913 \pm 1.0E-4	● 0.2302 \pm 2.6E-3	0.2354 \pm 2.3E-3	0.2339 \pm 2.7E-4
	MAE	0.1815 \pm 1.1E-6	0.2439 \pm 4.4E-5	0.2422 \pm 3.2E-5	0.1832 \pm 4.8E-5	0.4111 \pm 1.6E-2	● 0.1792 \pm 7.9E-5	0.1842 \pm 2.2E-4	0.1793 \pm 3.3E-4
D2	RMSE	1.0187 \pm 1.1E-6	1.1281 \pm 7.2E-3	1.1257 \pm 1.8E-4	1.0787 \pm 8.6E-7	1.8808 \pm 2.8E-2	1.1494 \pm 4.1E-5	1.0425 \pm 3.9E-4	1.0172 \pm 7.4E-4
	MAE	0.8079 \pm 2.5E-6	0.9256 \pm 1.5E-3	0.9229 \pm 1.9E-4	0.8580 \pm 6.2E-6	1.5403 \pm 2.6E-2	0.9257 \pm 2.1E-4	0.8014 \pm 4.9E-2	0.7856 \pm 7.9E-4
D3	RMSE	● 0.8665 \pm 7.8E-4	1.0336 \pm 5.4E-4	1.0848 \pm 5.3E-5	0.8713 \pm 3.7E-4	2.2963 \pm 9.8E-3	0.8845 \pm 1.1E-3	0.8982 \pm 4.4E-4	0.8675 \pm 8.2E-4
	MAE	0.6829 \pm 7.7E-6	0.8832 \pm 4.0E-4	0.9021 \pm 4.2E-5	0.6802 \pm 3.3E-4	1.9190 \pm 9.6E-3	0.7021 \pm 5.5E-3	0.7067 \pm 4.1E-4	0.6787 \pm 7.3E-4
D4	RMSE	0.8096 \pm 2.9E-6	¹ Failure	¹ Failure	¹ Failure	¹ Failure	0.8436 \pm 1.2E-3	0.8657 \pm 3.5E-4	0.8089 \pm 9.4E-4
	MAE	0.6221 \pm 7.9E-7	¹ Failure	¹ Failure	¹ Failure	¹ Failure	0.6530 \pm 4.9E-3	0.6650 \pm 2.9E-4	0.6193 \pm 5.1E-4
Win/Loss		7/1	8/0	8/0	8/0	8/0	6/2	8/0	-
Friedman Rank		2.5	6.38	6.13	4.38	7.63	3.75	3.88	1.38

¹Note that M2-M5 fails to achieve the final results on D4 on our experimental environment as shown in Table S12.

TABLE S14. Total time cost of M1-8 in RMSE/MAE on D1-4 (Secs), including Win/Loss counts and Friedman Rank

No.	CASE	M1	M2	M3	M4	M5	M6	M7	M8
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	87,425 \pm 9,048	46 \pm 4
	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	78,395 \pm 8,698	60 \pm 5
D2	RMSE	275 \pm 47	236 \pm 35	128 \pm 21	138 \pm 39	55 \pm 7	2,109 \pm 295	1,264 \pm 99	25 \pm 5
	MAE	308 \pm 39	32 \pm 3	128 \pm 27	766 \pm 64	56 \pm 6	2,256 \pm 633	1,156 \pm 286	29 \pm 8
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	9,921 \pm 2,586	26 \pm 6
	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	8,998 \pm 1,446	30 \pm 9
D4	RMSE	2,972 \pm 378	¹ Failure	¹ Failure	¹ Failure	¹ Failure	266,885 \pm 12,775	^a 1,644,502 \pm 98,039	334 \pm 46
	MAE	9,236 \pm 849	¹ Failure	¹ Failure	¹ Failure	¹ Failure	232,974 \pm 13,157	^a 997,259 \pm 84,311	358 \pm 31
Win/Loss		8/0	8/0	8/0	8/0	8/0	8/0	8/0	8/0
Friedman Rank		3.13	5	6	6.75	3.5	4.88	5.75	1

¹Note that M2-M5 fails to achieve the final results on D4 on our experimental environment as shown in Table S12.

TABLE S15. Results of the Wilcoxon signed-ranks test on RMSE/MAE of Table S13.

Comparison	<i>R</i>+	<i>R</i>-	¹<i>p</i>-value
M8 vs M1	34	2	0.0117
M8 vs M2	36	0	0.0039
M8 vs M3	36	0	0.0039
M8 vs M4	36	0	0.0039
M8 vs M5	36	0	0.0039
M8 vs M6	33	3	0.0195
M8 vs M7	36	0	0.0039

¹With a significance level of 0.1, the accepted hypotheses are highlighted.

TABLE S16. Results of the Wilcoxon signed-ranks test on time cost of Table S14.

Comparison	<i>R</i>+	<i>R</i>-	¹<i>p</i>-value
M8 vs M1	36	0	0.0039
M8 vs M2	36	0	0.0039
M8 vs M3	36	0	0.0039
M8 vs M4	36	0	0.0039
M8 vs M5	36	0	0.0039
M8 vs M6	36	0	0.0039
M8 vs M7	36	0	0.0039

¹With a significance level of 0.1, the accepted hypotheses are highlighted.