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^{2}NLF and additional figures are presented here.

I. Convergence of A^{2}NLF

A. Proof of Lemma 1

Note that learning objective of A^{2}NLF-PSO/A^{2}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 $a^t_{u,k(q)}$. Thus, it fulfills the following condition:

$$\lambda^t_{(q)}\left|\Lambda(u)\right|\left(p^t_{u,k(q)}-a^t_{u,k(q)}+\frac{h^{t-1}_{u,k(q)}}{\lambda^t_{(q)}\left|\Lambda(u)\right|}\right)=0. \tag{S1}$$

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

$$h^t_{u,k(q)}=\left(\eta^t_{(q)}-1\right)\lambda^t_{(q)}\left|\Lambda(u)\right|\left(p^t_{u,k(q)}-a^t_{u,k(q)}\right). \tag{S2}$$

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

$$\lambda^t_{(q)}\left|\Lambda(i)\right|\left(z^t_{i,k(q)}-x^t_{i,k(q)}+\frac{w^{t-1}_{i,k(q)}}{\lambda^t_{(q)}\left|\Lambda(i)\right|}\right)=0,\ \Rightarrow w^t_{i,k(q)}=\left(\eta^t_{(q)}-1\right)\lambda^t_{(q)}\left|\Lambda(i)\right|\left(z^t_{i,k(q)}-x^t_{i,k(q)}\right). \tag{S3}$$

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

B. Proof of Lemma 2

Considering the difference between $g\left(p^t_{u,k(q)},z^t_{i,k(q)},a^{t-1}_{u,k(q)},x^{t-1}_{i,k(q)},\psi^{t-1}_{2(q)}\right)$ and $g\left(\psi^{t-1}_{1(q)},\psi^{t-1}_{2(q)}\right)$, we have:

$$\begin{aligned}
&g\left(p^t_{u,k(q)},z^t_{i,k(q)},a^{t-1}_{u,k(q)},x^{t-1}_{i,k(q)},\psi^{t-1}_{2(q)}\right)-g\left(\psi^{t-1}_{1(q)},\psi^{t-1}_{2(q)}\right)\\
&\overset{(*)}{=}\left(\sum_{i\in\Lambda(u)}z^{t-1}_{i,k(q)}\left(y_{u,i}-\sum_{l_1=1}^{k-1}p^t_{u,l_1(q)}z^t_{i,l_1(q)}-p^t_{u,k(q)}z^{t-1}_{i,k(q)}-\sum_{l_2=k+1}^{d}p^{t-1}_{u,l_2(q)}z^{t-1}_{i,l_2(q)}\right)-\lambda^t_{(q)}\left|\Lambda(u)\right|\left(p^t_{u,k(q)}-a^{t-1}_{u,k(q)}+\frac{h^{t-1}_{u,k(q)}}{\lambda^t_{(q)}\left|\Lambda(u)\right|}\right)\right)\left(p^{t-1}_{u,k(q)}-p^t_{u,k(q)}\right)\\
&\quad+\left(\sum_{u\in\Lambda(i)}p^{t-1}_{u,k(q)}\left(y_{u,i}-\sum_{l_1=1}^{k-1}p^t_{u,l_1(q)}z^t_{i,l_1(q)}-p^{t-1}_{u,k(q)}z^t_{i,k(q)}-\sum_{l_2=k+1}^{d}p^{t-1}_{u,l_2(q)}z^{t-1}_{i,l_2(q)}\right)-\lambda^t_{(q)}\left|\Lambda(i)\right|\left(z^t_{i,k(q)}-x^{t-1}_{i,k(q)}+\frac{w^{t-1}_{i,k(q)}}{\lambda^t_{(q)}\left|\Lambda(i)\right|}\right)\right)\left(z^{t-1}_{i,k(q)}-z^t_{i,k(q)}\right)\\
&\quad-\frac{1}{2}\left(\sum_{i\in\Lambda(u)}\left(z^{t-1}_{i,k(q)}\right)^2+\lambda^t_{(q)}\left|\Lambda(u)\right|\right)\left(p^t_{u,k(q)}-p^{t-1}_{u,k(q)}\right)^2-\frac{1}{2}\left(\sum_{u\in\Lambda(i)}\left(p^{t-1}_{u,k(q)}\right)^2+\lambda^t_{(q)}\left|\Lambda(i)\right|\right)\left(z^t_{i,k(q)}-z^{t-1}_{i,k(q)}\right)^2.
\end{aligned} \tag{S4}$$

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

$$\begin{aligned}
&g\left(p_{u,k(q)}^{t},z_{i,k(q)}^{t},a_{u,k(q)}^{t-1},x_{i,k(q)}^{t-1},\psi_{2(q)}^{t-1}\right)-g\left(\psi_{1(q)}^{t-1},\psi_{2(q)}^{t-1}\right)\\
&=-\frac{1}{2}\left(\sum_{i\in\Lambda(u)}\left(z_{i,k(q)}^{t-1}\right)^{2}+\lambda_{(q)}^{t}\left|\Lambda(u)\right|\right)\left(p_{u,k(q)}^{t}-p_{u,k(q)}^{t-1}\right)^{2}-\frac{1}{2}\left(\sum_{u\in\Lambda(i)}\left(p_{u,k(q)}^{t-1}\right)^{2}+\lambda_{(q)}^{t}\left|\Lambda(i)\right|\right)\left(z_{i,k(q)}^{t}-z_{i,k(q)}^{t-1}\right)^{2}.
\end{aligned}\tag{S5}$$

Thus, the difference between $g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t-1}\right)$ and $g\left(p_{u,k(q)}^{t},z_{i,k(q)}^{t},a_{u,k(q)}^{t-1},x_{i,k(q)}^{t-1},\psi_{2(q)}^{t-1}\right)$ is:

$$g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t-1}\right)-g\left(p_{u,k(q)}^{t},z_{i,k(q)}^{t},a_{u,k(q)}^{t-1},x_{i,k(q)}^{t-1},\psi_{2(q)}^{t-1}\right)=-\left(\lambda_{(q)}^{t}\left|\Lambda(u)\right|/2\right)\left(a_{u,k(q)}^{t}-a_{u,k(q)}^{t-1}\right)^{2}-\left(\lambda_{(q)}^{t}\left|\Lambda(i)\right|/2\right)\left(x_{i,k(q)}^{t}-x_{i,k(q)}^{t-1}\right)^{2}.\tag{S6}$$

Moreover, $g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right)$ and $g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t-1}\right)$ yields:

$$\begin{aligned}
&g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right)-g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t-1}\right)\\
&=\left(p_{u,k(q)}^{t}-a_{u,k(q)}^{t}\right)\left(h_{u,k(q)}^{t}-h_{u,k(q)}^{t-1}\right)+\left(z_{i,k(q)}^{t}-x_{i,k(q)}^{t}\right)\left(w_{i,k(q)}^{t}-w_{i,k(q)}^{t-1}\right)\\
&\overset{\text{(I)}}{=}\frac{1}{\eta_{(q)}^{t}\lambda_{(q)}^{t}\left|\Lambda(u)\right|}\left(h_{u,k(q)}^{t}-h_{u,k(q)}^{t-1}\right)^{2}+\frac{1}{\eta_{(q)}^{t}\lambda_{(q)}^{t}\left|\Lambda(i)\right|}\left(w_{i,k(q)}^{t}-w_{i,k(q)}^{t-1}\right)^{2}\\
&\overset{\text{(II)}}{\le}\frac{2\left|\Lambda(u)\right|}{\eta_{(q)}^{t}\lambda_{(q)}^{t}}\left(\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}p_{u,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}p_{u,k(q)}^{t-1}\right)^{2}+\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}a_{u,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}a_{u,k(q)}^{t-1}\right)^{2}\right)\\
&+\frac{2\left|\Lambda(i)\right|}{\eta_{(q)}^{t}\lambda_{(q)}^{t}}\left(\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}z_{i,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}z_{i,k(q)}^{t-1}\right)^{2}+\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}x_{i,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}x_{i,k(q)}^{t-1}\right)^{2}\right),
\end{aligned}\tag{S7}$$

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:

$$\begin{aligned}
&g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right)-g\left(\psi_{1(q)}^{t-1},\psi_{2(q)}^{t-1}\right)\\
&\le-\frac{1}{2}\left(\sum_{i\in\Lambda(u)}\left(z_{i,k(q)}^{t-1}\right)^{2}+\lambda_{(q)}^{t}\left|\Lambda(u)\right|\right)\left(p_{u,k(q)}^{t}-p_{u,k(q)}^{t-1}\right)^{2}-\frac{\lambda_{(q)}^{t}\left|\Lambda(u)\right|}{2}\left(a_{u,k(q)}^{t}-a_{u,k(q)}^{t-1}\right)^{2}\\
&-\frac{1}{2}\left(\sum_{u\in\Lambda(i)}\left(p_{u,k(q)}^{t-1}\right)^{2}+\lambda_{(q)}^{t}\left|\Lambda(i)\right|\right)\left(z_{i,k(q)}^{t}-z_{i,k(q)}^{t-1}\right)^{2}-\frac{\lambda_{(q)}^{t}\left|\Lambda(i)\right|}{2}\left(x_{i,k(q)}^{t}-x_{i,k(q)}^{t-1}\right)^{2}\\
&+\frac{2\left|\Lambda(u)\right|}{\eta_{(q)}^{t}\lambda_{(q)}^{t}}\left(\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}p_{u,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}p_{u,k(q)}^{t-1}\right)^{2}+\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}a_{u,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}a_{u,k(q)}^{t-1}\right)^{2}\right)\\
&+\frac{2\left|\Lambda(i)\right|}{\eta_{(q)}^{t}\lambda_{(q)}^{t}}\left(\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}z_{i,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}z_{i,k(q)}^{t-1}\right)^{2}+\left(\left(\eta_{(q)}^{t}-1\right)\lambda_{(q)}^{t}x_{i,k(q)}^{t}-\left(\eta_{(q)}^{t-1}-1\right)\lambda_{(q)}^{t-1}x_{i,k(q)}^{t-1}\right)^{2}\right).
\end{aligned}\tag{S8}$$

Owing to (24a), (25a) stands, which indicates that the augmented Lagrangian function (3) related to $s_{(q)}$ or τ_q is non-increasing as $a_{u,k(q)}^{t}$>0 and $x_{i,k(q)}^{t}$>0. Then after the t-th iteration, the partial objective from (3) related to $s_{(q)}$ or τ_q is formulated as:

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

(S9)

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

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

(S10) indicates that if (24b) is fulfilled, (25b) holds, thereby making (3) related to $s_{(q)}$ or τ_q 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.□

C. Proof of Theorem 1

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

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

With (24), when (S1) is fulfilled, the upper-bound of $g\left(\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right)-g\left(\psi_{1(q)}^{t-1},\psi_{2(q)}^{t-1}\right)$ is zero as $t\rightarrow\infty$, thereby achieving (26). Following (S8) and (26), we have [24]:

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

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

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

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

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

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

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

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

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

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:

$$\begin{aligned}&\left(p_{u,k(q)}^{t-1}-p_{u,k(q)}^{t}\right)\left(\sum_{i\in\Lambda(u)}\left(z_{i,k(q)}^{t-1}\right)^2+\lambda_{(q)}^{t}\left|\Lambda(u)\right|\right)\\&=\sum_{i\in\Lambda(u)}z_{i,k(q)}^{t-1}\left(\sum_{l_1=1}^{k}p_{u,l_1(q)}^{t}z_{i,l_1(q)}^{t}+\sum_{l_2=k+1}^{d}p_{u,l_2(q)}^{t-1}z_{i,l_2(q)}^{t-1}-y_{u,i}\right)+\lambda_{(q)}^{t}\left|\Lambda(u)\right|\left(p_{u,k(q)}^{t-1}-a_{u,k(q)}^{t-1}\right)+h_{u,k(q)}^{t-1},\end{aligned}\tag{S14a}$$

$$\begin{aligned}&\left(z_{i,k(q)}^{t-1}-z_{i,k(q)}^{t}\right)\left(\sum_{u\in\Lambda(i)}\left(p_{i,k(q)}^{t-1}\right)^2+\lambda_{(q)}^{t}\left|\Lambda(i)\right|\right)\\&=\sum_{u\in\Lambda(i)}p_{u,k(q)}^{t-1}\left(\sum_{l_1=1}^{k}p_{u,l_1(q)}^{t}z_{i,l_1(q)}^{t}+\sum_{l_2=k+1}^{d}p_{u,l_2(q)}^{t-1}z_{i,l_2(q)}^{t-1}-y_{u,i}\right)+\lambda_{(q)}^{t}\left|\Lambda(i)\right|\left(z_{i,k(q)}^{t-1}-x_{i,k(q)}^{t-1}\right)+w_{i,k(q)}^{t-1}.\end{aligned}\tag{S14b}$$

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

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

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

Hence, considering a limit point $\left\{\psi_{1(q)}^{*},\psi_{2(q)}^{*}\right\}$ of a sequence $\left\{\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right\}$ 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):

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

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

$$p_{u,k}^{*}-a_{u,k}^{*}\to 0,\tag{S16c}$$

$$z_{i,k}^{*}-x_{i,k}^{*}\to 0.\tag{S16d}$$

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:

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

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

$$\begin{aligned}g_{(q)}=&\frac{1}{2}\sum_{y_{u,i}\in\Lambda}\left(y_{u,i}-\sum_{k=1}^{d}p_{u,k(q)}z_{i,k(q)}\right)^2+\sum_{(u,k)}h_{u,k(q)}\left(p_{u,k(q)}-a_{u,k(q)}\right)+\sum_{(u,k)}\frac{\lambda_{(q)}\left|\Lambda(u)\right|}{2}\left(p_{u,k(q)}-a_{u,k(q)}\right)^2\\&+\sum_{(i,k)}w_{i,k(q)}\left(z_{i,k(q)}-x_{i,k(q)}\right)+\sum_{(i,k)}\frac{\lambda_{(q)}\left|\Lambda(i)\right|}{2}\left(z_{i,k(q)}-x_{i,k(q)}\right)^2.\end{aligned}\tag{S18}$$

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

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

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]:

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

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

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

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^{2}NLF-PSO/A^{2}NLF-TPE are closely connected with the KKT conditions of its learning objective.

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

$$\left.\frac{\partial g^{\#}_{(q)}}{\partial a_{u,k(q)}}\right|_{a_{u,k(q)}=a^*_{u,k(q)}}=-\lambda^*_{(q)}\left|\Lambda(u)\right|\left(p^*_{u,k(q)}-a^*_{u,k(q)}+\frac{h^*_{u,k(q)}}{\lambda^*_{(q)}\left|\Lambda(u)\right|}\right)-m^*_{u,k(q)}=0,\tag{S22a}$$

$$m^*_{u,k(q)}a^*_{u,k(q)}=0,\tag{S22b}$$

$$a^*_{u,k(q)}\geq 0,\tag{S22c}$$

$$m^*_{u,k(q)}\geq 0,\tag{S22d}$$

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 $\{m^t_{u,k(q)}\}$ generated by the update rules of $m_{u,k}$ based on (S19). According to (S17)-(S21) and $a^t_{u,k(q)}=0$, conditions (S22a)-(S22c) are satisfied. Thus, we have:

$$m^*_{u,k(q)}=-\lambda^*_{(q)}\left|\Lambda(u)\right|\left(p^*_{u,k(q)}-a^*_{u,k(q)}+\frac{h^*_{u,k(q)}}{\lambda^*_{(q)}\left|\Lambda(u)\right|}\right).\tag{S23}$$

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

$$a^*_{u,k(q)}\leftarrow p^*_{u,k(q)}+\frac{h^*_{u,k(q)}}{\lambda^*_{(q)}\left|\Lambda(u)\right|}.\tag{S24}$$

By substituting (S24) into (S23), we have $m^*_{u,k(q)}=0$. Hence, conditions (S22c) and (S22d) are fulfilled. Note that as $x^t_{i,k(q)}>0$ 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. □

D. Proof of Lemma 3

The difference between $g\left(p^{t}_{u,k(q)},z^{t}_{i,k(q)},a^{t-1}_{u,k(q)},x^{t-1}_{i,k(q)},\psi^{t-1}_{2(q)}\right)$ and $g\left(\psi^{t-1}_{1(q)},\psi^{t-1}_{2(q)}\right)$ in this case is also given by (S5). Considering the fact of $a^{t}_{u,k(q)}$=0 and, $x^{t}_{i,k(q)}$>0 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:

$$g\left(\psi^{t}_{1(q)},\psi^{t-1}_{2(q)}\right)-g\left(p^{t}_{u,k(q)},z^{t}_{i,k(q)},a^{t-1}_{u,k(q)},x^{t-1}_{i,k(q)},\psi^{t-1}_{2(q)}\right)=-\frac{\lambda^{t}_{(q)}\left|\Lambda(u)\right|}{2}\left(a^{t-1}_{u,k(q)}\right)^{2}-\frac{\lambda^{t}_{(q)}\left|\Lambda(i)\right|}{2}\left(x^{t}_{i,k(q)}-x^{t-1}_{i,k(q)}\right)^{2}. \tag{S25}$$

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:

$$\begin{aligned}
&g\left(\psi^{t}_{1(q)},\psi^{t}_{2(q)}\right)-g\left(\psi^{t}_{1(q)},\psi^{t-1}_{2(q)}\right)\\
&=\left(p^{t}_{u,k(q)}-a^{t}_{u,k(q)}\right)\left(h^{t}_{u,k(q)}-h^{t-1}_{u,k(q)}\right)+\left(z^{t}_{i,k(q)}-x^{t}_{i,k(q)}\right)\left(w^{t}_{i,k(q)}-w^{t-1}_{i,k(q)}\right)\\
&\overset{(\mathrm{I})}{=}\eta^{t}_{(q)}\lambda^{t}_{(q)}\left|\Lambda(u)\right|\left(p^{t}_{u,k(q)}-a^{t}_{u,k(q)}\right)^{2}+\frac{1}{\eta^{t}_{(q)}\lambda^{t}_{(q)}\left|\Lambda(i)\right|}\left(w^{t}_{i,k(q)}-w^{t-1}_{i,k(q)}\right)^{2}\\
&\overset{(\mathrm{II})}{\le}\eta^{t}_{(q)}\lambda^{t}_{(q)}\left|\Lambda(u)\right|\left(p^{t}_{u,k(q)}\right)^{2}+\frac{2\left|\Lambda(i)\right|}{\eta^{t}_{(q)}\lambda^{t}_{(q)}}\left(\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}z^{t}_{i,k(q)}-\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}z^{t-1}_{i,k(q)}\right)^{2}+\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}x^{t}_{i,k(q)}-\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}x^{t-1}_{i,k(q)}\right)^{2}\right),
\end{aligned} \tag{S26}$$

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 $a^{t}_{u,k(q)}$=0. With (S5), (S25) and (S26), we have the following deduction:

$$\begin{aligned}
&g\left(\psi^{t}_{1(q)},\psi^{t}_{2(q)}\right)-g\left(\psi^{t-1}_{1(q)},\psi^{t-1}_{2(q)}\right)\\
&\le-\frac{1}{2}\left(\sum_{i\in\Lambda(u)}\left(z^{t-1}_{i,k(q)}\right)^{2}+\lambda^{t}_{(q)}\left|\Lambda(u)\right|\right)\left(p^{t}_{u,k(q)}-p^{t-1}_{u,k(q)}\right)^{2}-\frac{\lambda^{t}_{(q)}\left|\Lambda(u)\right|}{2}\left(a^{t-1}_{u,k(q)}\right)^{2}\\
&\quad-\frac{1}{2}\left(\sum_{u\in\Lambda(i)}\left(p^{t-1}_{u,k(q)}\right)^{2}+\lambda^{t}_{(q)}\left|\Lambda(i)\right|\right)\left(z^{t}_{i,k(q)}-z^{t-1}_{i,k(q)}\right)^{2}-\frac{\lambda^{t}_{(q)}\left|\Lambda(i)\right|}{2}\left(x^{t}_{i,k(q)}-x^{t-1}_{i,k(q)}\right)^{2}\\
&\quad+\eta^{t}_{(q)}\lambda^{t}_{(q)}\left|\Lambda(u)\right|\left(p^{t}_{u,k(q)}\right)^{2}+\frac{2\left|\Lambda(i)\right|}{\eta^{t}_{(q)}\lambda^{t}_{(q)}}\left(\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}z^{t}_{i,k(q)}-\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}z^{t-1}_{i,k(q)}\right)^{2}+\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}x^{t}_{i,k(q)}-\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}x^{t-1}_{i,k(q)}\right)^{2}\right).
\end{aligned} \tag{S27}$$

Owing to (29), (25a) stands, which indicates that the augmented Lagrangian function (3) related to $s_{(q)}$ or τ_q is non-increasing as $a^{t}_{u,k(q)}$=0 and $x^{t}_{i,k(q)}$>0 in this case. Then after the *t*-th iteration, we substitute $a^{t}_{u,k(q)}$=0 into (S10):

$$\begin{aligned}
g\left(\psi^{t}_{1(q)},\psi^{t}_{2(q)}\right)=&\frac{1}{2}\sum_{y_{u,i}\in\Lambda}\left(y_{u,i}-\sum_{l_1=1}^{k}p^{t}_{u,l_1(q)}z^{t}_{i,l_1(q)}-\sum_{l_2=k+1}^{d}p^{t-1}_{u,l_2(q)}z^{t-1}_{i,l_2(q)}\right)^{2}\\
&+\sum_{u}\left|\Lambda(u)\right|\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}\left(\sum_{l_1=1}^{k-1}\left(p^{t}_{u,l_1(q)}-a^{t}_{u,l_1(q)}\right)^{2}+\left(p^{t}_{u,k(q)}\right)^{2}\right)+\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}\sum_{l_2=k+1}^{d}\left(p^{t-1}_{u,l_2(q)}-a^{t-1}_{u,l_2(q)}\right)^{2}\right)\\
&+\sum_{i}\left|\Lambda(i)\right|\left(\left(\eta^{t}_{(q)}-1\right)\lambda^{t}_{(q)}\sum_{l_1=1}^{k}\left(z^{t}_{i,l_1(q)}-x^{t}_{i,l_1(q)}\right)^{2}+\left(\eta^{t-1}_{(q)}-1\right)\lambda^{t-1}_{(q)}\sum_{l_2=k+1}^{d}w^{t}_{i,l_2(q)}\left(z^{t-1}_{i,l_2(q)}-x^{t-1}_{i,l_2(q)}\right)^{2}\right)\\
&+\sum_{u}\frac{\lambda^{t}_{(q)}\left|\Lambda(u)\right|}{2}\left(\sum_{l_1=1}^{k-1}\left(p^{t}_{u,l_1(q)}-a^{t}_{u,l_1(q)}\right)^{2}+\left(p^{t}_{u,k(q)}\right)^{2}+\sum_{l_2=k+1}^{d}\left(p^{t-1}_{u,l_2(q)}-a^{t-1}_{u,l_2(q)}\right)^{2}\right)\\
&+\sum_{i}\frac{\lambda^{t}_{(q)}\left|\Lambda(i)\right|}{2}\left(\sum_{l_1=1}^{k}\left(z^{t}_{i,l_1(q)}-x^{t}_{i,l_1(q)}\right)^{2}+\sum_{l_2=k+1}^{d}\left(z^{t-1}_{i,l_2(q)}-x^{t-1}_{i,l_2(q)}\right)^{2}\right).
\end{aligned} \tag{S28}$$

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

E. Proof of Theorem 2

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

$$\lim_{t\to\infty} a_{u,k(q)}^{t-1} \to 0, \tag{S29a}$$

$$\lim_{t\to\infty} p_{u,k(q)}^{t} \to 0. \tag{S29b}$$

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

Part b. Firstly, considering a limit point $\left\{\psi_{1(q)}^{*},\psi_{2(q)}^{*}\right\}$ of a sequence $\left\{\psi_{1(q)}^{t},\psi_{2(q)}^{t}\right\}$ 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 $a_{u,k(q)}^{t}$=0, and $x_{i,k(q)}^{t}$>0 in this case. Then considering the KKT conditions related to $a_{u,k(q)}$, i.e., (S22).

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

$$p_{u,k(q)}^{*} + \frac{h_{u,k(q)}^{*}}{\lambda_{(q)}^{*}\left|\Lambda(u)\right|} \le 0. \tag{S30}$$

Note that (S30) indicates that:

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

Thus, condition (S22) are all fulfilled in this case. 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* 2 stands, and **Step 5** is implemented. ■

II. Additional Figures

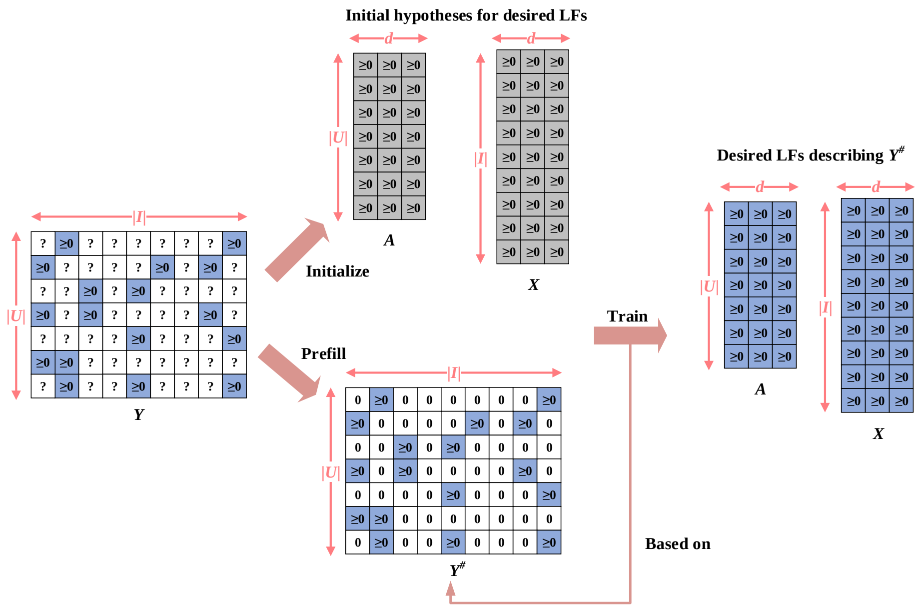


Fig. S1. Processing flow of an NMF model.

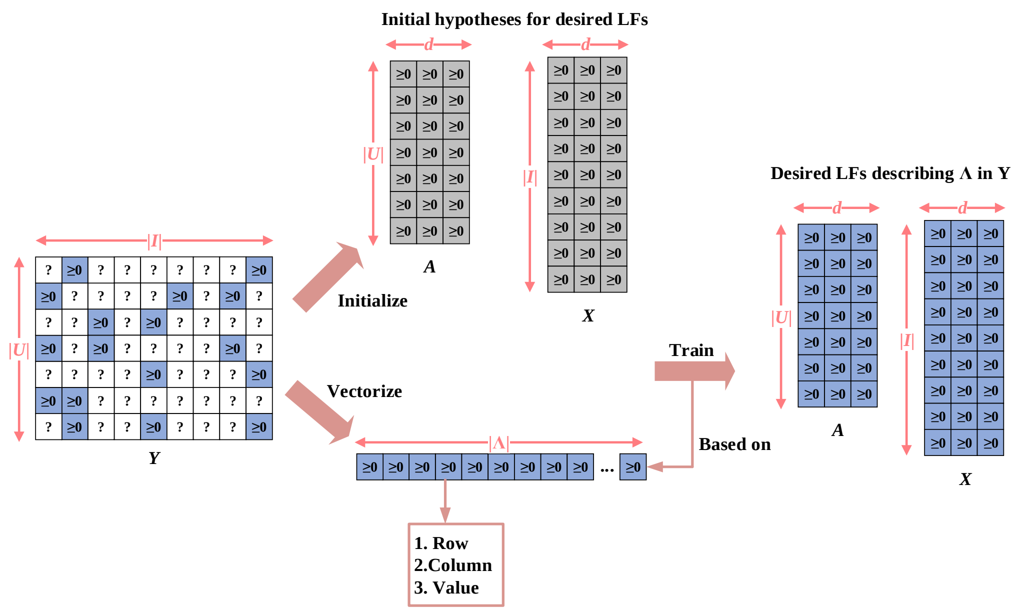
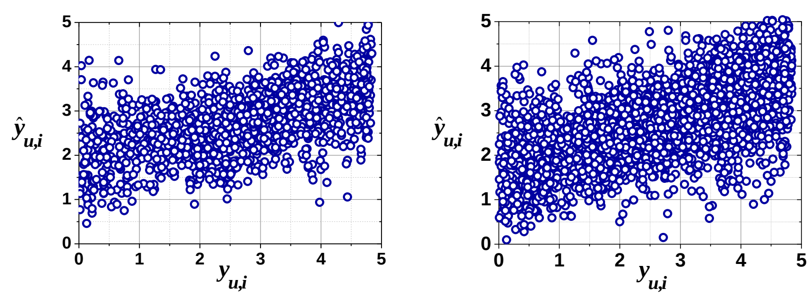


Fig. S2. Processing flow of an NLFA model.



(a) A^{2}NLF-PSO (b) A^{2}NLF-TPE

Fig. S3. Relations between $y_{u,i}$ in Λ and corresponding $\hat{y}_{u,i}$ generated by an A^{2}NLF-PSO/A^{2}NLF-TPE model on D2 as d=20.

III. Additional Tables

TABLE S.I. Grid-search Range of Hyper-parameters in M1-8 on D1-4.

No.	Hyper-parameters	Grid-searching Range
M1	Augmentation coefficient λ	$2^{-6}, 2^{-4}, \ldots, 2^{8}$
	Learning rate η	$8, 4, 2, 1, 2^{-1}, 2^{-2}, 2^{-3}$
M2	Penalty coefficient λ	2, 1.8, …, 0.8
M3	Regularization coefficient μ	$8, 4, 2, 1, 2^{-1}, 2^{-2}, 2^{-3}$
	L_p coefficient p	1.2, 1.3, …, 2.0
M4	Penalty coefficient α	$1, 10, \ldots, 10^{5}$
	Penalty coefficient β	$10, 10^{2}, \ldots, 10^{6}$
M5	Penalty coefficient ρ	$2^{-3}, 2^{-5}, \ldots, 2^{-17}$
M6	Regularization coefficient λ	$10^{-6}, 5\times10^{-5}, \ldots, 10^{-3}$
	Learning rate η	$10^{-5}, 5\times10^{-4}, \ldots, 10^{-2}$
	Batch size bs	$2^{5}, 2^{6}, 2^{7}, 2^{8}, 2^{9}, 2^{10}$
M7	Regularization coefficient λ	$10^{-5}, 5\times10^{-4}, \ldots, 10^{-2}$
	Learning rate η	$10^{-5}, 5\times10^{-4}, \ldots, 10^{-2}$
	Batch size bs	$2^{8}, 2^{9}, 2^{10}, 2^{11}, 2^{12}, 2^{13}$
M8	Regularization coefficient λ	$10^{-6}, 5\times10^{-5}, \ldots, 10^{-3}$
	Learning rate η	$10^{-6}, 5\times10^{-5}, \ldots, 10^{-3}$
	Batch size bs	$2^{11}, 2^{12}, 2^{13}, 2^{14}, 2^{15}, 2^{16}$

TABLE S.II. 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.III. 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

[1]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.IV. 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

[1]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.V. 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

[1]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.VI. Optimal Hyper-parameters during M5's Ten Times' Training Process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-5}$
	MAE	$\rho=2^{-7}$	$\rho=2^{-5}$	$\rho=2^{-7}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-7}$	$\rho=2^{-5}$	$\rho=2^{-5}$	$\rho=2^{-7}$	$\rho=2^{-5}$
D2	RMSE	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-15}$	$\rho=2^{-15}$	$\rho=2^{-13}$
	MAE	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-15}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-15}$
D3	RMSE	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$
	MAE	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-13}$	$\rho=2^{-13}$	$\rho=2^{-15}$	$\rho=2^{-15}$	$\rho=2^{-13}$
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

[1]M5 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.VII. Optimal Hyper-parameters during M6's Ten Times' Training Process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\lambda=10^{-4}$, $\eta=5\times10^{-3}$, [1]bs=2^9	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-4}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-4}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^9
	MAE	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9
D2	RMSE	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-1}$, $\eta=5\times10^{-3}$, bs=2^6	$\lambda=10^{-1}$, $\eta=5\times10^{-3}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-1}$, $\eta=5\times10^{-3}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-1}$, $\eta=5\times10^{-3}$, bs=2^6	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^6
	MAE	$\lambda=10^{-4}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-3}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-4}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-3}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-4}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-4}$, $\eta=10^{-2}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^6
D3	RMSE	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^7
	MAE	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-5}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^7
D4	RMSE	$\lambda=10^{-3}$, $\eta=10^{-4}$, bs=2^9	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-4}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=10^{-4}$, bs=2^9	$\lambda=10^{-5}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=10^{-4}$, bs=2^9	$\lambda=10^{-5}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-3}$, $\eta=10^{-4}$, bs=2^9
	MAE	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-5}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=10^{-3}$, bs=2^9	$\lambda=10^{-2}$, $\eta=5\times10^{-3}$, bs=2^9

[1]The abbreviation 'bs' denotes the batch size adopted by M6 on an HDI matrix.

TABLE S.VIII. Optimal Hyper-parameters during M7's Ten Times' Training Process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\lambda=10^{-3}$, $\eta=10^{-3}$, [1]bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}
	MAE	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}
D2	RMSE	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}
	MAE	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{10}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{10}
D3	RMSE	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}
	MAE	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{11}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{11}
D4	RMSE	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-2}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}
	MAE	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=5\times10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=5\times10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=5\times10^{-3}$, bs=2^{12}	$\lambda=10^{-3}$, $\eta=10^{-3}$, bs=2^{12}

[1]The abbreviation 'bs' denotes batch size adopted by M7 on an HDI matrix.

TABLE S.IX. Optimal Hyper-parameters during M8's Ten Times' Training Process on D1-4

No.	Type	1	2	3	4	5	6	7	8	9	10
D1	RMSE	$\lambda=10^{-4}$, $\eta=10^{-4}$, [1]bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}
	MAE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=5\times10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-5}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}
D2	RMSE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=10^{-5}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}
	MAE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-5}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}
D3	RMSE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=10^{-5}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}
	MAE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{13}	$\lambda=5\times10^{-4}$, $\eta=10^{-5}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{13}
D4	RMSE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}
	MAE	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=5\times10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}	$\lambda=10^{-4}$, $\eta=10^{-4}$, bs=2^{14}

[1]The abbreviation 'bs' denotes batch size adopted by M7 on an HDI matrix.

TABLE S.X. RMSE, MAE and Time Cost of M1, M9 and M10 on D1-4.

Dataset	Model	Case	Prediction Accuracy	[1]Tuning Time Cost (Secs)	[2]Testing Time Cost (Secs)	Total Time Cost (Secs)
D1	M1	RMSE	0.2373±2.2E-6	428±22.7	6±2.4	434±25
		MAE	0.1815±1.1E-6	439±25.4	6±2.8	445±28
	M9	RMSE	**0.2339±2.7E-4**	-	-	**46±4**
		MAE	**0.1793±3.3E-4**	-	-	**60±5**
	M10	RMSE	0.2573±1.4E-6	-	-	387±33
		MAE	0.2015±2.8E-6	-	-	396±46
D2	M1	RMSE	1.0187±1.1E-6	271±45.4	4±1.7	275±47
		MAE	0.8079±2.5E-6	305±38.3	3±0.9	308±39
	M9	RMSE	**1.0158±6.4E-4**	-	-	**25±5**
		MAE	**0.7848±9.3E-4**	-	-	**29±8**
	M10	RMSE	1.0209±2.0E-5	-	-	87±11
		MAE	0.7883±1.3E-5	-	-	85±9
D3	M1	RMSE	**0.8665±7.8E-4**	739±72.3	21±14.7	759±87
		MAE	0.6829±1.7E-6	756±53.8	3±0.5	763±54
	M9	RMSE	0.8673±1.3E-3	-	-	**26±6**
		MAE	**0.6785±9.6E-5**	-	-	**30±9**
	M10	RMSE	0.8684±4.7E-4	-	-	487±59
		MAE	0.6793±2.8E-5	-	-	268±40
D4	M1	RMSE	0.8096±2.9E-6	2,934±353.8	38±24.6	3,972±378
		MAE	0.6221±7.9E-7	9,203±828.9	33±20.4	9,236±849
	M9	RMSE	0.8091±3.0E-3	-	-	**334±46**
		MAE	**0.6191±1.7E-4**	-	-	**358±31**
	M10	RMSE	**0.8086±6.0E-5**	-	-	3731±311
		MAE	0.6199±7.1E-6	-	-	5532±566

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

TABLE S.XI. Results of the Wilcoxon Signed-ranks Test for M9 on RMSE/MAE of Table S.IX

Comparison	*R+*	*R-*	[1]*p-value*
M9 vs M1	34	2	**0.0234**
M9 vs M2	36	0	**0.0078**
M9 vs M3	36	0	**0.0078**
M9 vs M4	36	0	**0.0078**
M9 vs M5	36	0	**0.0078**
M9 vs M6	33	3	**0.0391**
M9 vs M7	36	0	**0.0078**
M9 vs M8	36	0	**0.0078**

[1]With a significance level of 0.05, the accepted hypotheses are highlighted.

TABLE S.XII. Results of the Wilcoxon Signed-ranks Test for M10 on RMSE/MAE of Table S.IX

Comparison	*R+*	*R-*	[1]*p-value*
M10 vs M1	20.5	15.5	0.7656
M10 vs M2	36	0	**0.0078**
M10 vs M3	36	0	**0.0078**
M10 vs M4	29	7	0.1484
M10 vs M5	36	0	**0.0078**
M10 vs M6	30	6	0.1094
M10 vs M7	29.5	6.5	0.1172
M10 vs M8	36	0	**0.0078**

[1]With a significance level of 0.05, the accepted hypotheses are highlighted.

TABLE S.XIII. Results of the Wilcoxon Signed-ranks Test for M9 on Total Time Cost of Table S.X

Comparison	*R+*	*R-*	[1]*p-value*
M9 vs M1	36	0	**0.0078**
M9 vs M2	36	0	**0.0078**
M9 vs M3	36	0	**0.0078**
M9 vs M4	36	0	**0.0078**
M9 vs M5	36	0	**0.0078**
M9 vs M6	36	0	**0.0078**
M9 vs M7	36	0	**0.0078**
M9 vs M8	36	0	**0.0078**

[1]With a significance level of 0.05, the accepted hypotheses are highlighted.

TABLE S.XIV. Results of the Wilcoxon Signed-ranks Test for M10 on Total Time Cost of Table S.X

Comparison	***R+***	***R-***	[1]***p-value***
M10 vs M1	36	0	**0.0078**
M10 vs M2	35	1	**0.0156**
M10 vs M3	36	0	**0.0078**
M10 vs M4	36	0	**0.0078**
M10 vs M5	33	3	**0.0391**
M10 vs M6	36	0	**0.0078**
M10 vs M7	36	0	**0.0078**
M10 vs M8	36	0	**0.0078**

[1]With a significance level of 0.05, the accepted hypotheses are highlighted.