## A Fine-Grained Regularization Scheme for Nonnegative Latent Factorization of High-Dimensional and Incomplete Tensors Supplementary File

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## I. INTRODUCTION

This is the supplementary file for paper entitled "A Fine-Grained Regularization Scheme for Nonnegative Latent Factorization of High-Dimensional and Incomplete Tensors", which presents the convergence proof of the proposed FRNL model and the work flow of predicting potential links via FRNL.

## II. Convergence Proof of FRNL

Considering the nonnegative constraints for latent feature matrices S, D, and T and linear bias vectors a, b, and c, we have the Lagrangian function L for (6) as:

$$L = \varepsilon \left( \mathbf{S}, \mathbf{D}, \mathbf{T}, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \right) - \sum_{i=1}^{|I|} \sum_{r=1}^{R} \tilde{s}_{ir} s_{ir} - \sum_{j=1}^{|I|} \sum_{r=1}^{R} \tilde{d}_{jr} d_{jr} - \sum_{k=1}^{|K|} \sum_{r=1}^{R} \tilde{t}_{kr} t_{kr} - \sum_{i=1}^{|I|} \tilde{a}_{i} a_{i} - \sum_{j=1}^{|I|} \tilde{b}_{j} b_{j} - \sum_{k=1}^{|K|} \tilde{c}_{k} c_{k}.$$
 (S1)

where  $\tilde{S}$ ,  $\tilde{D}$ ,  $\tilde{T}$   $\tilde{a}$ ,  $\tilde{b}$ , and  $\tilde{c}$  denote Lagrangian multipliers for S, D, T, a, b, and c.

Considering the partial derivatives of L with latent feature and linear bias, they are highly similar for S, D, T and a, b, c. Hence, we consider the case of  $s_{ir}$  and  $a_i$  as follows:

$$\begin{cases} \frac{\partial L}{\partial s_{ir}} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -d_{jr} t_{kr} \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}) - \tilde{s}_{ir} = 0, \\ \frac{\partial L}{\partial a_{i}} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -1 \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}) - \tilde{a}_{i} = 0. \end{cases} \Rightarrow \begin{cases} \tilde{s}_{ir} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -d_{jr} t_{kr} \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}), \\ \tilde{a}_{i} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -1 \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}). \end{cases}$$
(S2)

where  $\varphi(\theta) = p(\beta \theta^p e^{-\beta \theta} + \theta^{p-1} + \theta^{p-1} e^{-\beta \theta}) / (1 + e^{-\beta \theta})^{p+1}$ . Then, considering the KKT conditions of (S1), i.e.,  $\forall s_{ir}$ ,  $\tilde{s_{ir}}$ :  $s_{ir}\tilde{s_{ir}} = 0$ , and  $\forall a_i$ ,  $\tilde{a_i}$ :  $a_i\tilde{a_i} = 0$ , we have:

$$\begin{cases}
s_{ir} \left( \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -d_{jr} t_{kr} \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}) \right) = 0, \\
a_{i} \left( \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -1 \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}) \right) = 0.
\end{cases} \Rightarrow \begin{cases}
s_{ir} \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr} = s_{ir} \left( \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}) \right), \\
a_{i} \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} = a_{i} \left( \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}) \right).
\end{cases} (S3)$$

With (S3), we conveniently achieve the iterative learning rules given in (16). Hence, an SLF-NMU-based learning scheme in an FRNL model is closely connected to the KKT conditions of its learning objective. From this point of view, we theoretically prove the convergence of FRNL in the following two steps:

**Step 1:** The objective function (6) is non-increasing and lower-bounded.

**Step 2:** FRNL is guaranteed to converge at a KKT stationary point of its learning objective with the SFR scheme and SLF-NMU-based learning rules.

To implement Step 1, we present the following *Lemma* 1.

Lemma 1. With the following definitions,

$$\tau_{1} = \begin{pmatrix} \left(s_{ir}^{n+1} - s_{ir}^{n}\right)^{2} \left(\sum_{y_{ijk} \in \Lambda(i)} \left(d_{jr}^{n} t_{kr}^{n}\right)^{2} + \gamma \left|\Lambda(i)\right|^{\alpha} \Upsilon\left(s_{ir}^{n+1}\right)\right) + \left(a_{i}^{n+1} - a_{i}^{n}\right)^{2} \left(\left|\Lambda(i)\right| + \gamma \left|\Lambda(i)\right|^{\alpha} \Upsilon\left(a_{i}^{n+1}\right)\right) + \left(d_{jr}^{n+1} - d_{jr}^{n}\right)^{2} \left(\sum_{y_{ijk} \in \Lambda(j)} \left(s_{ir}^{n+1} t_{kr}^{n}\right)^{2} + \gamma \left|\Lambda(j)\right|^{\alpha} \Upsilon\left(d_{jr}^{n+1}\right)\right) + \left(t_{jr}^{n+1} - t_{jr}^{n}\right)^{2} \left(\left|\Lambda(j)\right| + \gamma \left|\Lambda(j)\right|^{\alpha} \Upsilon\left(b_{j}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\sum_{y_{ijk} \in \Lambda(k)} \left(s_{ir}^{n+1} d_{jr}^{n+1}\right)^{2} + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(t_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left(c_{kr}^{n+1}\right)\right) + \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2} \left(\left|\Lambda(k)\right| + \gamma \left|\Lambda(k)\right|^{\alpha} \Upsilon\left$$

and

$$\tau_{2} = \left( \left( s_{ir}^{n+1} - s_{ir}^{n} \right)^{2} \gamma \left| \Lambda(i) \right|^{\alpha} \Psi(s_{ir}^{n+1}) + \left( a_{i}^{n+1} - a_{i}^{n} \right)^{2} \gamma \left| \Lambda(i) \right|^{\alpha} \Psi(a_{i}^{n+1}) + \left( d_{jr}^{n+1} - d_{jr}^{n} \right)^{2} \gamma \left| \Lambda(j) \right|^{\alpha} \Psi(d_{jr}^{n+1}) + \left( b_{j}^{n+1} - b_{j}^{n} \right)^{2} \gamma \left| \Lambda(j) \right|^{\alpha} \Psi(b_{j}^{n+1}) + \left( t_{kr}^{n+1} - t_{kr}^{n} \right)^{2} \gamma \left| \Lambda(k) \right|^{\alpha} \Psi(t_{kr}^{n+1}) + \left( c_{k}^{n+1} - c_{k}^{n} \right)^{2} \gamma \left| \Lambda(k) \right|^{\alpha} \Psi(c_{k}^{n+1}) \right) \right)$$

where  $\Upsilon(\theta) = p \left( (p-1)\theta^{p-2} \left( 1 + e^{-\beta\theta} \right)^2 + \beta \theta^{p-1} e^{-\beta\theta} \left( p + 2pe^{-\beta\theta} + 1 \right) + p\beta^2 \theta^p e^{-2\beta\theta} \right) / \left( 1 + e^{-\beta\theta} \right)^{p+2}$  and  $\Psi(\theta) = p\beta^2 \theta^p e^{-\beta\theta} / \left( 1 + e^{-\beta\theta} \right)^{p+2}$ .

if  $\tau_1 \ge \tau_2$ , then the following inequality holds:

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n+1}, a_{i}^{n+1}, b_{j}^{n+1}, c_{k}^{n+1}\right) - \varepsilon\left(s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) \le 0.$$
(S4)

Moreover, if  $\gamma \ge 0$ , we constantly have:

$$\varepsilon\left(s_{ir}^{n}, d_{ir}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{i}^{n}, c_{k}^{n}\right) \ge 0. \tag{S5}$$

Proof of *Lemma* 1. Firstly, considering the difference between  $\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n},t_{kr}^{n},a_{i}^{n},b_{j}^{n},c_{k}^{n}\right)$  and  $\varepsilon\left(s_{ir}^{n},d_{jr}^{n},t_{kr}^{n},a_{i}^{n},b_{j}^{n},c_{k}^{n}\right)$ , we have:

$$\varepsilon \left( s_{ir}^{n+1}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n} \right) - \varepsilon \left( s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n} \right) \\
\triangleq \left( \sum_{y_{ijk} \in \Lambda(i)} \left( y_{ijk} - \left( \sum_{r=1}^{R} s_{ir}^{n+1} d_{jr}^{n} t_{kr}^{n} + a_{i}^{n} + b_{j}^{n} + c_{k}^{n} \right) \right) \left( -d_{jr}^{n} t_{kr}^{n} \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi \left( s_{ir}^{n+1} \right) \right) \left( s_{ir}^{n+1} - s_{ir}^{n} \right) \\
- \frac{1}{2} \left( \sum_{y_{ijk} \in \Lambda(i)} \left( d_{jr}^{n} t_{kr}^{n} \right)^{2} + \gamma \left| \Lambda(i) \right|^{\alpha} \left( \Upsilon \left( s_{ir}^{n+1} \right) + \Psi \left( s_{ir}^{n+1} \right) \right) \right) \left( s_{ir}^{n+1} - s_{ir}^{n} \right)^{2}.$$
(S6)

where  $\triangleq$  denotes the second-order approximation of a function. Based on SLF-NMU, considering  $s_{ir}$ 's optimal condition [63], (S6) is reformulated as:

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) - \varepsilon\left(s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) = -\frac{1}{2} \left(\sum_{y_{nk} \in \Lambda(i)} \left(d_{jr}^{n} t_{kr}^{n}\right)^{2} + \gamma \left|\Lambda(i)\right|^{\alpha} \left(\Upsilon\left(s_{ir}^{n+1}\right) + \Psi\left(s_{ir}^{n+1}\right)\right)\right) \left(s_{ir}^{n+1} - s_{ir}^{n}\right)^{2}. \tag{S7}$$

Similarly, we have:

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) - \varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) = -\frac{1}{2} \left(\sum_{y_{jk} \in \Lambda(j)} \left(s_{ir}^{n+1} t_{kr}^{n}\right)^{2} + \gamma \left|\Lambda(j)\right|^{\alpha} \left(\Upsilon\left(d_{jr}^{n+1}\right) + \Psi\left(d_{jr}^{n+1}\right)\right)\right) \left|d_{jr}^{n+1} - d_{jr}^{n}\right|^{2}.$$
(S8)

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n+1}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) - \varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) = -\frac{1}{2} \left(\sum_{y_{ijk} \in \Lambda(k)} \left(s_{ir}^{n+1} d_{jr}^{n+1}\right)^{2} + \gamma \left|\Lambda(k)\right|^{\alpha} \left(\Upsilon\left(t_{kr}^{n+1}\right) + \Psi\left(t_{kr}^{n+1}\right)\right)\right) \left(t_{kr}^{n+1} - t_{kr}^{n}\right)^{2}.$$
 (S9)

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n+1}, a_{i}^{n+1}, b_{j}^{n}, c_{k}^{n}\right) - \varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n+1}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) = -\frac{1}{2} \left(\left|\Lambda\left(i\right)\right| + \gamma \left|\Lambda\left(i\right)\right|^{\alpha} \left(\Upsilon\left(a_{i}^{n+1}\right) + \Psi\left(a_{i}^{n+1}\right)\right)\right) \left(a_{i}^{n+1} - a_{i}^{n}\right)^{2}. \tag{S10}$$

$$\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n+1},t_{kr}^{n+1},a_{i}^{n+1},b_{j}^{n+1},c_{k}^{n}\right)-\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n+1},t_{kr}^{n+1},a_{i}^{n+1},b_{j}^{n},c_{k}^{n}\right)=-\frac{1}{2}\left(\left|\Lambda\left(j\right)\right|+\gamma\left|\Lambda\left(j\right)\right|^{\alpha}\left(\Upsilon\left(b_{j}^{n+1}\right)+\Psi\left(b_{j}^{n+1}\right)\right)\right)\left(b_{j}^{n+1}-b_{j}^{n}\right)^{2}.\tag{S11}$$

$$\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n+1},t_{kr}^{n+1},a_{i}^{n+1},b_{j}^{n+1},c_{k}^{n+1}\right)-\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n+1},t_{kr}^{n+1},a_{i}^{n+1},b_{j}^{n+1},c_{k}^{n}\right)=-\frac{1}{2}\left(\left|\Lambda\left(k\right)\right|+\gamma\left|\Lambda\left(k\right)\right|^{\alpha}\left(\Upsilon\left(c_{k}^{n+1}\right)+\Psi\left(c_{k}^{n+1}\right)\right)\right)\left(c_{k}^{n+1}-c_{k}^{n}\right)^{2}. \tag{S12}$$

With (S7)-(S12), we have:

$$\begin{split} &\varepsilon\left(s_{ir}^{n+1},d_{jr}^{n+1},t_{kr}^{n+1},a_{i}^{n+1},b_{j}^{n+1},c_{k}^{n+1}\right)-\varepsilon\left(s_{ir}^{n},d_{jr}^{n},t_{kr}^{n},a_{i}^{n},b_{j}^{n},c_{k}^{n}\right)=\\ &-\frac{1}{2}\Biggl(\sum_{y_{ijk}\in\Lambda(i)}\left(d_{jr}^{n}t_{kr}^{n}\right)^{2}+\gamma\left|\Lambda\left(i\right)\right|^{\alpha}\left(\Upsilon\left(s_{ir}^{n+1}\right)+\Psi\left(s_{ir}^{n+1}\right)\right)\Biggr)\left(s_{ir}^{n+1}-s_{ir}^{n}\right)^{2}-\frac{1}{2}\Biggl(\left|\Lambda\left(i\right)\right|+\gamma\left|\Lambda\left(i\right)\right|^{\alpha}\left(\Upsilon\left(a_{i}^{n+1}\right)+\Psi\left(a_{i}^{n+1}\right)\right)\Biggr)\left(a_{i}^{n+1}-a_{i}^{n}\right)^{2}\\ &-\frac{1}{2}\Biggl(\sum_{y_{ijk}\in\Lambda(j)}\left(s_{ir}^{n+1}t_{kr}^{n}\right)^{2}+\gamma\left|\Lambda\left(j\right)\right|^{\alpha}\left(\Upsilon\left(d_{jr}^{n+1}\right)+\Psi\left(d_{jr}^{n+1}\right)\right)\Biggr)\left(d_{jr}^{n+1}-d_{jr}^{n}\right)^{2}-\frac{1}{2}\Biggl(\left|\Lambda\left(j\right)\right|+\gamma\left|\Lambda\left(j\right)\right|^{\alpha}\left(\Upsilon\left(b_{j}^{n+1}\right)+\Psi\left(b_{j}^{n+1}\right)\right)\Biggr)\left(b_{j}^{n+1}-b_{j}^{n}\right)^{2}\\ &-\frac{1}{2}\Biggl(\sum_{y_{ijk}\in\Lambda(k)}\left(s_{ir}^{n+1}d_{jr}^{n+1}\right)^{2}+\gamma\left|\Lambda\left(k\right)\right|^{\alpha}\left(\Upsilon\left(t_{kr}^{n+1}\right)+\Psi\left(t_{kr}^{n+1}\right)\right)\Biggr)\left(t_{kr}^{n+1}-t_{kr}^{n}\right)^{2}-\frac{1}{2}\Biggl(\left|\Lambda\left(k\right)\right|+\gamma\left|\Lambda\left(k\right)\right|^{\alpha}\left(\Upsilon\left(c_{k}^{n+1}\right)+\Psi\left(c_{k}^{n+1}\right)\right)\Biggr)\left(c_{k}^{n+1}-c_{k}^{n}\right)^{2}. \end{split} \tag{S13}$$

Hence, if  $\tau_1 \ge \tau_2$ , the following inequality evidently holds:

$$\varepsilon\left(s_{ir}^{n+1}, d_{jr}^{n+1}, t_{kr}^{n+1}, a_{i}^{n+1}, b_{j}^{n+1}, c_{k}^{n+1}\right) - \varepsilon\left(s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) \le 0. \tag{S14}$$

Thus, the objective function (6) is non-increasing

Moreover, after the *n*-th iteration, (6) is formulated as:

$$\mathcal{E}\left(s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) \\
= \frac{1}{2} \sum_{y_{ijk} \in \Lambda} \left( y_{ijk} - \left( \sum_{r=1}^{R} s_{ir}^{n} d_{jr}^{n} t_{kr}^{n} + a_{i}^{n} + b_{j}^{n} + c_{k}^{n} \right) \right)^{2} \\
+ \gamma \sum_{i=1}^{|I|} |\Lambda(i)|^{\alpha} \left( \sum_{r=1}^{R} \left( \frac{s_{ir}^{n}}{1 + e^{-\beta s_{ir}}} \right)^{p} + \left( \frac{a_{i}^{n}}{1 + e^{-\beta a_{i}}} \right)^{p} \right) \\
+ \gamma \sum_{j=1}^{|I|} |\Lambda(j)|^{\alpha} \left( \sum_{r=1}^{R} \left( \frac{d_{jr}^{n}}{1 + e^{-\beta d_{jr}}} \right)^{p} + \left( \frac{b_{j}^{n}}{1 + e^{-\beta b_{j}}} \right)^{p} \right) \\
+ \gamma \sum_{k=1}^{|K|} |\Lambda(k)|^{\alpha} \left( \sum_{r=1}^{R} \left( \frac{t_{kr}^{n}}{1 + e^{-\beta t_{kr}}} \right)^{p} + \left( \frac{c_{k}^{n}}{1 + e^{-\beta c_{k}}} \right)^{p} \right). \tag{S15}$$

From (S15), we see that if  $\gamma \ge 0$  is satisfied, the following inequality must be true:

$$\varepsilon\left(s_{ir}^{n}, d_{jr}^{n}, t_{kr}^{n}, a_{i}^{n}, b_{j}^{n}, c_{k}^{n}\right) \ge 0. \tag{S16}$$

Hence, the objective function (6) is low-bounded. According to the above inferences, *Lemma* 1 holds. Therefore, it can be proven that the objective function (6) is non-increasing and lower-bounded. Then to implement Step 2, we present the following *Theorem* 1.

**Theorem 1.** Sequences  $\left\{s_{ir}^n, d_{jr}^n, t_{kr}^n, a_i^n, b_j^n, c_k^n\right\}$  learnt from update rules in (17) converge to a stationary point  $\left\{s_{ir}^*, d_{jr}^*, t_{kr}^*, a_i^*, b_j^*, c_k^*\right\}$  of  $\varepsilon\left(s_{ir}, d_{jr}, t_{kr}, a_i, b_j, c_k\right)$  in (6).

Note that the proof process of  $\{s_{ir}^n, d_{jr}^n, t_{kr}^n\}$  is similar and  $\{a_i^n, b_j^n, c_k^n\}$  is also similar, hence, for conciseness, we only present the proof with  $\{s_{ir}^n\}$  and  $\{a_i^n\}$ .

*Proof of Theorm* 1. Firstly, based on (S4) and (S5),  $\forall i \in I, j \in J, k \in K$ , we have the following references [67]:

$$\lim_{n \to +\infty} \left( s_{ir}^{n+1} - s_{ir}^{n} \right) = 0, \lim_{n \to +\infty} \left( a_{i}^{n+1} - a_{i}^{n} \right) = 0, 
\lim_{n \to +\infty} \left( d_{jr}^{n+1} - d_{jr}^{n} \right) = 0, \lim_{n \to +\infty} \left( b_{j}^{n+1} - b_{j}^{n} \right) = 0, 
\lim_{n \to +\infty} \left( t_{kr}^{n+1} - t_{kr}^{n} \right) = 0, \lim_{n \to +\infty} \left( c_{k}^{n+1} - c_{k}^{n} \right) = 0.$$
(S17)

From (S14) we see that a sequence  $\{s_{ir}^n\}$  converges with the update rule (17). Let  $\{s_{ir}^*\}$  denotes the converging state of  $\{s_{ir}^n\}$ , i.e.,  $0 \le s_{ir}^* = \lim_{n \to +\infty} s_{ir}^n < +\infty$ . Then for the objective (6), the following KKT conditions related to  $\{s_{ir}^n\}$  should be fulfilled if  $\{s_{ir}^*\}$  is one of its stationary point.

$$\left. \frac{\partial L}{\partial s_{ir}} \right|_{s_{ir} = s_{ir}^*} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -d_{jr} t_{kr} \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(\tilde{s}_{ir}^*) - \tilde{s}_{ir}^* = 0, \tag{S18a}$$

$$\tilde{s}_{ir}^* \cdot s_{ir}^* = 0, \tag{S18b}$$

$$s_{ir}^* \ge 0, \tag{S18c}$$

$$\tilde{s}_{i}^* \ge 0.$$
 (S18d)

Note that following (S1)-(S3), condition (S18a) is evidently fulfilled with parameter update rule (17), making the following equation holds:

$$\tilde{s}_{ir}^* = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -d_{jr} t_{kr} \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(\tilde{s}_{ir}^*), \tag{S19}$$

Hence, we focus on analyzing condition (S18c) and (S18d). We first construct  $\xi_{ir}^n$  as:

$$\xi_{ir}^{n} = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr}}{\sum_{x_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir})}.$$
 (S20)

Naturally, (S20) is bounded by non-negative si:

$$0 \le \xi_{ir}^* = \lim_{n \to +\infty} \xi_{ir}^n = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr}}{\sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}^*)}.$$
 (S21)

Thus, we write the update rule of sir with SLF-NMU as:

$$S_{ir}^{n+1} = S_{ir}^{n} \xi_{ir}^{n}. \tag{S22}$$

By combining (S17) and (S22), we have:

$$\lim_{n \to +\infty} \left( s_{ir}^{n+1} - s_{ir}^{n} \right) = 0 \Rightarrow s_{ir}^{*} \xi_{ir}^{*} - s_{ir}^{*} = 0.$$
 (S23)

Note that following the update rule (17),  $s_{ir}^* \ge 0$  with a non-negatively initial hypothesis. Hence, we have the following inferences.

a) **When**  $s_{ir}^* > 0$ . Based on (S20) and (S23), we have:

$$\lim_{n \to +\infty} s_{ir}^* \xi_{ir}^* - s_{ir}^* = 0, s_{ir}^* > 0 \Rightarrow \xi_{ir}^* = 1 \Rightarrow \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}^*) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr} = 0.$$
(S24)

By combing (S19) and (S24), we achieve condition (S18b):

$$\tilde{s}_{ir}^* = \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}^*) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr} = 0 \Rightarrow \tilde{s}_{ir}^* \cdot s_{ir}^* = 0.$$
 (S25)

Meanwhile, when  $\tilde{s}_{ir}^* = 0$  and  $s_{ir}^* > 0$ , condition (S18c) and (S18d) are naturally fulfilled. Hence, when  $s_{ir}^* > 0$ , KKT conditions in (S18) are all satisfied.

b) When  $s_{ir}^*$  =0. The conditions (S18b) and (S18c) naturally holds. Hence, we only need to justify that whether condition (S18d) is fulfilled or not. To do so, we reformulate  $s_{ir}^*$  as follows:

$$s_{ir}^* = s_{ir}^0 \lim_{n \to +\infty} \prod_{h=1}^n \xi_{ir}^h. \tag{S26}$$

Based on (S26) we further have the following deduction:

$$s_{ir}^{0} > 0, s_{ir}^{0} \lim_{n \to +\infty} \prod_{h=1}^{n} \xi_{ir}^{h} = s_{ir}^{*} = 0 \Rightarrow \lim_{n \to +\infty} \prod_{h=1}^{n} \xi_{ir}^{h} = 0$$

$$\Rightarrow \lim_{n \to +\infty} \xi_{ir}^{n} = \xi_{ir}^{*} = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr}}{\sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}^{*})} \leq 1$$

$$\Rightarrow \tilde{s}_{ir}^{*} = \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} d_{jr} t_{kr} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(s_{ir}^{*}) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} d_{jr} t_{kr} \geq 0.$$
(S27)

Hence, the condition (S18d) holds. Therefore, when  $s_{ir}^* = 0$ , KKT conditions in (S18) are all satisfied.

By analogy, we can prove that sequences  $\{d_{jr}^n\}$  and  $\{t_{kr}^n\}$  converge to a stationary point of (6), too. Next, we prove the convergence of sequence  $\{a_i^n\}$ .

Let  $a_i^*$  denotes the converging state of sequence  $\{a_i^n\}$ , i.e.,  $\forall i \in I : 0 \le a_i^* = \lim_{n \to +\infty} a_i^n \le +\infty$ . If  $a_i^*$  is one of  $a_i^n$ 's stationary point, the following KKT conditions should be fulfilled:

$$\left. \frac{\partial L}{\partial a_i} \right|_{a_i = a_i^*} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -1 \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_i^*) - \tilde{a}_i^* = 0, \tag{S28a}$$

$$\tilde{a}_i^* \cdot a_i^* = 0. \tag{S28b}$$

$$a_i^* \ge 0,$$
 (S28c)

$$\tilde{a}_i^* \ge 0. \tag{S28d}$$

Following (S1)-(S3), we see that condition (S28a) naturally holds. Hence, we have:

$$\tilde{a}_{i}^{*} = \sum_{y_{ijk} \in \Lambda(i)} \left( \left( y_{ijk} - \hat{y}_{ijk} \right) \left( -1 \right) \right) + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*}). \tag{S29}$$

Thus, we focus on condition (S28c) and (S28d), we first construct  $\zeta_i^n$  as follows:

$$\zeta_{i}^{n} = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk}}{\sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*})}.$$
(S30)

Obviously, (S30) is bounded by non-negative  $a_i^n$ , hence, we have:

$$0 \le \varsigma_{i}^{*} = \lim_{n \to +\infty} \varsigma_{i}^{n} = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk}}{\sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*})}.$$
(S31)

Accordingly, the update rule of  $a_i^n$  can be rewrite as:

$$a_i^{n+1} = a_i^n \varsigma_i^n \tag{S32}$$

By combining (S17) and (S32), we have:

$$\lim_{n \to +\infty} \left( a_i^{n+1} - a_i^n \right) = 0 \Rightarrow a_i^* \varsigma_i^* - a_i^* = 0.$$
 (S33)

Note that following the update rule (17),  $a_i^* \ge 0$  with a non-negatively initial hypothesis. Hence, we have the following inferences.

a) **When**  $a_i^* > 0$ . Based on (S30) and (S33), we have:

$$a_{i}^{*}\varsigma_{i}^{*} - a_{i}^{*} = 0, a_{i}^{*} \ge 0 \Rightarrow \varsigma_{i}^{*} = 1 \Rightarrow \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*}) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} = 0.$$
(S34)

By combing (S29) and (S34), we achieve condition (S28b):

$$\tilde{a}_{i}^{*} = \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*}) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} = 0 \Rightarrow \tilde{a}_{i}^{*} \cdot a_{i}^{*} = 0.$$
(S35)

Meanwhile, when  $a_i^* > 0$  and  $\tilde{a}_i^* = 0$ , conditions (S28c) and (S28d) naturally hold. Therefore, when  $a_i^* > 0$ , KKT conditions in (S28) are all satisfied.

b) **When**  $a_i^*$ =0. Under such circumstance, conditions (S28b) and (S28c) are naturally fulfilled. Thus, we need to justify that whether condition (S28d) is fulfilled or not. To this end, we formulated  $\tilde{a}_i^*$  as follows:

$$a_i^* = a_i^0 \lim_{n \to +\infty} \prod_{i=1}^n \zeta_i^h.$$
 (S36)

Following (S36), we have:

$$a_{i}^{0} > 0, a_{i}^{0} \lim_{n \to +\infty} \prod_{h=1}^{n} \varsigma_{i}^{h} = a_{i}^{*} = 0 \Rightarrow \lim_{n \to +\infty} \prod_{h=1}^{n} \varsigma_{i}^{h} = 0$$

$$\Rightarrow \lim_{n \to +\infty} \varsigma_{i}^{n} = \varsigma_{i}^{*} = \frac{\sum_{y_{ijk} \in \Lambda(i)} y_{ijk}}{\sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*})} \leq 1$$

$$\Rightarrow \tilde{a}_{i}^{*} = \sum_{y_{ijk} \in \Lambda(i)} \hat{y}_{ijk} + \gamma \left| \Lambda(i) \right|^{\alpha} \varphi(a_{i}^{*}) - \sum_{y_{ijk} \in \Lambda(i)} y_{ijk} \geq 0.$$
(S37)

Hence, when  $a_i^* = 0$ , KKT conditions in (S28) are also satisfied. Therefore, based on the above inference, *Theorem* 1 stands. As a result, it can be proven that FRNL is guaranteed to converge at a KKT stationary point of its learning objective. According to Theorem 1, Step 2 is implemented. By combining steps 1-2, we conclude that with the SLF-NMU-based learning scheme (17), an FRNL model's convergence on a nonnegative HDI tensor is guaranteed.

## III. THE FLOW OF PREDICTING POTENTIAL LINKS VIA FRNL

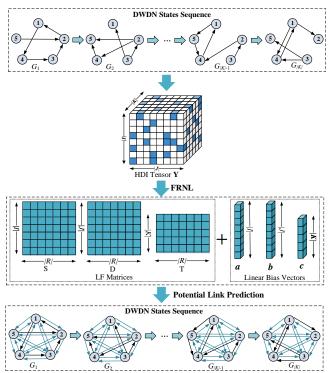


Fig. S1. Predicting potential links via FRNL on a DWDN.