Heterogeneous graph inference based on similarity network fusion for predicting lncRNA-miRNA interaction

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Theorem 1. When ***WL*** and ***WM*** are properly normalized utilizing formula (2) and formula (3) respectively, it is guaranteed that formula (1) will converge.

$$W_{i+1} = \lambda WL \times W_i \times WM + (1-\lambda) W_0 \tag{1}$$

$$WL(l_i, l_j) = \frac{WL(l_i, l_j)}{\sqrt{\sum_{n=1}^{nl} WL(l_i, l_n)}\sqrt{\sum_{n=1}^{nl} WL(l_j, l_n)}} \tag{2}$$

$$WM(m_i, m_j) = \frac{WM(m_i, m_j)}{\sqrt{\sum_{n=1}^{nm} WM(m_i, m_n)}\sqrt{\sum_{n=1}^{nm} WM(m_j, m_n)}} \tag{3}$$

Proof of Theorem 1

In this section, we denote *WL*, *WM* and *W* to *A*, *B* and *X* respectively. *A is* $nl \times nl$ matrices , *B* is $nm \times nm$ matrices and *X* is $nl \times nm$ matrices. Besides, we denote A_i and A^j as the i-th row of *A* and j-th column of *A* respectively. a_{ij} is used to represent the value of $A(i,j)$. We use the similar way to define the matrix *B* and *X*.

After that, according to formula (1), we can obtain:

$$x_{ij} = \lambda A_i X B^j + (1-\lambda) x_{ij}^0 \tag{4}$$

For X^1, we can also get:

$$\begin{bmatrix} x_{1,1} \\ \vdots \\ x_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} a_{1,1}b_{1,1},\cdots,a_{1,n}b_{1,1},\cdots,a_{1,1}b_{m,1},\cdots,a_{1,n}b_{m,1} \\ \vdots \\ a_{n,1}b_{1,1},\cdots,a_{n,n}b_{1,1},\cdots,a_{n,1}b_{m,1},\cdots,a_{n,n}b_{m,1} \end{bmatrix} \begin{bmatrix} x_{1,1} \\ \vdots \\ x_{n,1} \\ \vdots \\ x_{1,m} \\ \vdots \\ x_{n,m} \end{bmatrix} + (1-\lambda) \begin{bmatrix} x^{0}_{1,1} \\ \vdots \\ x^{0}_{n,1} \end{bmatrix} \quad (5)$$

If we use $A_i \times B^j$ to denote $\begin{bmatrix} a_{i,1}b_{1,j} & \cdots & a_{i,n}b_{1,j} & \cdots & a_{i,1}b_{m,j} & \cdots & a_{i,n}b_{m,j} \end{bmatrix}$ and then formula (1) can be written as:

$$\begin{bmatrix} X^1 \\ \vdots \\ X^m \end{bmatrix} = \lambda \begin{bmatrix} A_1 \times B^1 \\ \vdots \\ A_n \times B^1 \\ \vdots \\ A_1 \times B^m \\ \vdots \\ A_n \times B^m \end{bmatrix} \begin{bmatrix} X^1 \\ \vdots \\ X^m \end{bmatrix} + (1-\lambda) \begin{bmatrix} X^{10} \\ \vdots \\ X^{m0} \end{bmatrix} \quad (6)$$

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

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

By comparing the above two equations, we can find that *C* is a $nl \times nm$ symmetrical matrix. We use X^* to represents $\begin{bmatrix} X^1 & \cdots & X^n \end{bmatrix}^{\mathrm{T}}$, the formula (6) can be written:

$$X^* = \lambda C X^* + (1-\lambda) X^{*0} \quad (7)$$

In order to get a converged solution for formula (7), *C* can be normalized as $C^{norm} = D^{-1/2} C D^{-1/2}$, where *D* is a diagonal matrix with $d_{i,i}$ equals to the sum of the i-th row of *C*. Hence, we can also get $c^{norm}_{i,j} = \frac{c_{i,j}}{\sqrt{d_{i,i} d_{j,j}}}$ and $d_{i,i} = \sum_{u=1}^{nm} c_{i,u} = \sum_{u=1}^{nm} a_{t,\theta_u} b_{r_u+1,s+1} = \sum_{p=1}^{n} a_{t,p} \sum_{q=1}^{m} b_{q,s+1}$ where $u = r_u n + \theta_u$. After incorporating the above equation into $c^{norm}_{i,j}$, we can obtain:

$$c_{i,j}^{norm} = \frac{a_{t,\theta} b_{r+1,s+1}}{\sqrt{\sum_{p=1}^{n} a_{t,p} \sum_{q=1}^{m} b_{q,s+1}} \sqrt{\sum_{p=1}^{n} a_{\theta,p} \sum_{q=1}^{m} b_{q,r+1}}} = \frac{a_{t,\theta}}{\sqrt{\sum_{p=1}^{n} a_{t,p} \sum_{p=1}^{n} a_{\theta,p}}} \frac{b_{r+1,s+1}}{\sqrt{\sum_{q=1}^{m} b_{q,s+1} \sum_{q=1}^{m} b_{q,r+1}}} \quad (8)$$

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

We can get $c_{i,j}^{norm} = a_{t,\theta}^{norm} b_{r+1,s+1}^{norm}$. Thus, we can rewrite formula (7) as $X^* = \lambda C^{norm} X^* + (1-\lambda) X^{*0}$.