

Supplementary Materials

1. Derivation of solution for common W matrix:

Suppose \mathbf{X}^i , $i=1, 2, \dots, m$ be matrices representing m types of genomic assays profiled on same set of n samples with p_i features, \mathbf{W} be the common basis matrix, \mathbf{H}^i , $i=1, \dots, m$ be the individual data specific coefficient matrices and $\theta^i \geq 0$, $i=1, \dots, m$ be the weights for several data types. Then we can write

$$\mathbf{X}_{n \times p_i}^i \approx \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i \quad i = 1, 2, \dots, m$$

Where $\mathbf{W}_{n \times k} \geq 0$, $\mathbf{H}_{k \times p_i}^i \geq 0$, $i = 1, 2, \dots, m$

The intNMF problem minimizes the following objective function

$$Q = \sum_{i=1}^m \theta^i (\mathbf{X}_{n \times p_i}^i - \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i)^2$$
$$Q = \sum_{i=1}^m [\sqrt{\theta^i} (\mathbf{X}_{n \times p_i}^i - \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i)]^2$$

There is no global minimum solution for NMF problem. Therefore, it is unrealistic to design an algorithm to find the global minimum of Q . We derive approximate solution for \mathbf{W} . Since our objective is to approximately factorize $\mathbf{X}_{n \times p_i}^i$ in to $\mathbf{W}_{n \times k}$ and $\mathbf{H}_{k \times p_i}^i$ matrices for $i=1, 2, \dots, m$, and that each of the m terms in the above equation is strictly positive we can write,

$$\sqrt{\theta^i} (\mathbf{X}_{n \times p_i}^i - \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i) \approx \mathbf{0}_{n \times p_i}$$

$$\sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i \approx \sqrt{\theta^i} \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i$$

For simplicity, writing the expression in the form of equation

$$\sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i = \sqrt{\theta^i} \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i + \mathbf{C}_{n \times p_i}^i$$

Where $\mathbf{C}_{n \times p_i}^i$ is matrix of constants having small numbers.

Multiplying both sides by transpose of $\mathbf{H}_{k \times p_i}^i$ and summing over i

$$\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} = \sum_{i=1}^m \sqrt{\theta^i} \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} + \sum_{i=1}^m \mathbf{C}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k}$$

$$\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} = \sum_{i=1}^m \sqrt{\theta^i} \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} + \mathbf{C}'_{n \times k}$$

Where, $\mathbf{C}'_{n \times k} = \sum_{i=1}^m \mathbf{C}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k}$ is a constant. Note that \mathbf{H}^i , $i=1, \dots, m$ are computed separately.

$$\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} = \mathbf{W}_{n \times k} \sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} + \mathbf{C}'_{n \times k}$$

$$\mathbf{W}_{n \times k} = \left(\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right) \left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^{-1} - \mathbf{C}'_{n \times k} \left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^{-1}$$

$$\mathbf{W}_{k \times n}^T = \left[\left(\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right) \left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^{-1} \right]^T + \mathbf{C}''_{k \times n}$$

Where $\mathbf{C}''_{k \times n} = \left[-\mathbf{C}'_{n \times k} \left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^{-1} \right]^T$ constant matrix. Writing back in approximate form,

$$\mathbf{W}_{k \times n}^T \approx \left[\left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^T \right]^{-1} \left[\left(\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right)^T \right]$$

This equation can be solved using non negative alternating least square method. Finally $\mathbf{W}_{n \times k}$ is obtained by the transpose of $\mathbf{W}_{k \times n}^T$.

2. Solution for H matrices

\mathbf{H}^i , $i=1, \dots, m$ matrices are solved using non-negativity constraint least square method.

$$\mathbf{H}_{k \times p_i}^i \approx (\mathbf{W}^T \mathbf{W})_{k \times k}^{-1} \mathbf{W}_{k \times n}^T \mathbf{X}_{n \times p_i}^i \quad i = 1, 2, \dots, m$$

such that $\mathbf{H}_{k \times p_i}^i \geq 0$

3. Convergence of intNMF to standard NMF when $m \rightarrow 1$

For, $i=1, \dots, m$ the solution for W is given by

$$\mathbf{W}_{k \times n}^T \approx \left[\left(\sum_{i=1}^m \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^T \right]^{-1} \left[\left(\sum_{i=1}^m \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right)^T \right]$$

If $m \rightarrow 1$,

$$\mathbf{W}_{k \times n}^T \approx \left[\left(\sum_{i=1}^1 \sqrt{\theta^i} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^T \right]^{-1} \left[\left(\sum_{i=1}^1 \sqrt{\theta^i} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right)^T \right]$$

There is no need of weight for a single data. i.e. $\theta^i \rightarrow 1$

$$\begin{aligned} \mathbf{W}_{k \times n}^T &\approx \left[\left(\sum_{i=1}^1 \sqrt{1} (\mathbf{H}^i (\mathbf{H}^i)^T)_{k \times k} \right)^T \right]^{-1} \left[\left(\sum_{i=1}^1 \sqrt{1} \mathbf{X}_{n \times p_i}^i (\mathbf{H}^i)^T_{p_i \times k} \right)^T \right] \\ &= [(\mathbf{H}^1 (\mathbf{H}^1)^T)_{k \times k}]^{-1} [(\mathbf{X}_{n \times p_1}^1 (\mathbf{H}^1)^T_{p_1 \times k})^T] \\ &= (\mathbf{H}^1 (\mathbf{H}^1)^T)_{k \times k}^{-1} \mathbf{H}_{k \times p_1}^1 (\mathbf{X}^1)_{p_1 \times n}^T \end{aligned}$$

Which is solution of

$$\begin{aligned} (\mathbf{X}^1)_{p_1 \times n}^T &\approx (\mathbf{H}^1)_{p_1 \times k}^T \mathbf{W}_{k \times n}^T \\ \Rightarrow \mathbf{X}_{n \times p_1}^1 &\approx \mathbf{W}_{n \times k} \mathbf{H}_{k \times p_1}^1 \end{aligned}$$

For simplicity, writing p for p_1 , \mathbf{X} for \mathbf{X}^1 and \mathbf{H} for \mathbf{H}^1 .

$$\mathbf{X}_{n \times p} \approx \mathbf{W}_{n \times k} \mathbf{H}_{k \times p}$$

Which is standard NMF problem.

(Complete set of supplementary figures are provided separately with **S2 File. Complete set of Supplementary Figures**).