Relationship with nonnegative matrix factorization

First, for ease of explanation, let assume that the full representation \( L = 1 \) is used. Suppose that each \( m \) has unique appropriate index from 1 to \( |M| = \prod_{l=1}^{L} M_l \) (the number of possible mutation patterns), so that \( m \) can be indices of matrices.

Let \( G = \{g_i,m\} \) denote the \( I \times |M| \) matrix, where \( g_i,m \) is the number of mutations whose mutation patterns are equal to \( m \) in the \( i \)-th cancer genome. Nonnegative matrix factorization aims to find low rank decomposition, \( G \sim \tilde{Q}F \), where \( \tilde{Q} = \{\tilde{q}_{i,k}\} \) and \( F = \{f_k,m\} \) are nonnegative matrix, and row vectors of \( F \) are often restricted to be sum to one. We used the notation \( \tilde{Q} \) instead of \( Q \) to represent that the row vectors of \( \tilde{Q} \) are not normalized to sum to one in general.

For solving NMF, the previous study (Lee et al. 2000) used the following updating rule:

\[
\begin{align*}
    f_{k,m} &\leftarrow f_{k,m} \frac{(\tilde{Q}^T G)_{k,m}}{(\tilde{Q}^T \tilde{Q}F)_{k,m}}, \\
    \tilde{q}_{i,k} &\leftarrow \tilde{q}_{i,k} \frac{(GF^T)_{i,k}}{(\tilde{Q}FF^T)_{i,k}},
\end{align*}
\]

that reduces the Euclidean distance \( ||G - \tilde{Q}F|| \). Therefore, the optimization problem for the existing approach is

\[
\begin{align*}
    \text{minimize} & \quad ||G - \tilde{Q}F|| \\
    \text{subject to} & \quad \sum_m f_{k,m} = 1, \quad k = 1, \ldots, K \\
    & \quad f_{k,m} \geq 0, \quad k = 1, \ldots, K, \quad m \in M \\
    & \quad \tilde{q}_{i,k} \geq 0, \quad i = 1, \ldots, I, \quad k = 1, \ldots, K.
\end{align*}
\] (1)

On the other hand, there is another type of updating rule:

\[
\begin{align*}
    f_{k,m} &\leftarrow f_{k,m} \frac{\sum_i \tilde{q}_{i,k} g_{i,m}}{\sum_i \tilde{q}_{i,k}}, \\
    \tilde{q}_{i,k} &\leftarrow \tilde{q}_{i,k} \frac{\sum_m f_{k,m} g_{i,m}}{\sum_m f_{k,m}},
\end{align*}
\]

that reduces the Kullback-Liebler Divergence:

\[
KL(G||\tilde{Q}F) = \sum_{i,m} \left( g_{i,m} \log \frac{g_{i,m}}{(QF)_{i,m}} - g_{i,m} + (\tilde{Q}f)_{i,m} \right).
\]

In general cases including the independent representation, there is restrictions \( f_{k,m} = \prod_l f_{k,l,m_l} \) by smaller set of parameters. Let us consider the following optimization problem with the Kullback-Liebler Divergence and the restrictions on \( F \):

\[
\begin{align*}
    \text{minimize} & \quad KL(G||\tilde{Q}F) \\
    \text{subject to} & \quad f_{k,m} = \prod_l f_{k,l,m_l}, \quad k = 1, \ldots, K, \quad m \in M \\
    & \quad f_{k,l,p} \geq 0, \quad k = 1, \ldots, K, \quad m \in M \\
    & \quad \tilde{q}_{i,k} \geq 0, \quad i = 1, \ldots, I, \quad k = 1, \ldots, K.
\end{align*}
\] (2)

In fact, this is equivalent to the proposed method, whose optimization problem can be written as:

\[
\begin{align*}
    \text{maximize} & \quad L(Q,F|G)(= \sum_{i,m} g_{i,m} \log (QF)_{i,m}) \\
    \text{subject to} & \quad f_{k,m} = \prod_l f_{k,l,m_l}, \quad k = 1, \ldots, K, \quad m \in M \\
    & \quad f_{k,l,p} \geq 0, \quad k = 1, \ldots, K, \quad m \in M \\
    & \quad \sum_k q_{i,k} = 1, \quad i = 1, \ldots, I \\
    & \quad q_{i,k} \geq 0, \quad i = 1, \ldots, I, \quad k = 1, \ldots, K.
\end{align*}
\] (3)
**Proposition 1** When \((Q,F) = (Q^*, F^*)\) is an optimal solution of the optimization problem \((\mathcal{Q}, \mathcal{F})\), then \((\tilde{Q}, F) = (R^*Q^*, F^*)\) is an optimal solution of the optimization problem \((\tilde{\mathcal{Q}}, \mathcal{F})\). On the other hand, when \((\tilde{Q}, F) = (\tilde{Q}^*, F^*)\) is an optimal solution of the optimization problem \((\tilde{\mathcal{Q}}, \mathcal{F})\), then \((Q,F) = (R^*^{-1}\tilde{Q}^*, F^*)\) is an optimal solution of the optimization problem \((\mathcal{Q}, \mathcal{F})\), where 

\[ R^* = \text{diag}(r_1^*, \ldots, r_I^*) \]

\[ r_i^* = \sum_m g_{i,m} \]

Proof. This is because

\[
KL(G||\tilde{Q}F) = -\sum_i \left( (\sum_m g_{i,m}) \log \tilde{r}_i - \tilde{r}_i \right) - L(Q, F|G) + \text{(constant value)},
\]

where \(Q\) is row-normalized matrix for \(\tilde{Q}\), \(\tilde{r}_i = \sum_k q_{i,k}\) for each \(i\), and \((\sum_m g_{i,m}) \log \tilde{r}_i - \tilde{r}_i\) takes its maximum at \(\tilde{r}_i = r_i^*\). \(\square\)