# On the Identifiability of Transform Learning for Non-negative Matrix Factorization (Supplementary Material) 

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## A. Proof of Lemma 1

To show that $c(\mathbf{\Phi}, \mathbf{W}, \mathbf{H}) \geq c\left(\overline{\boldsymbol{\Phi}}, \mathbf{W}^{*}, \mathbf{H}^{*}\right)$, we first minimize $c$ with respect to $\mathbf{W}, \mathbf{H}$. For a fixed orthogonal $\boldsymbol{\Phi} \in \mathbb{R}^{M \times M}$ we have

$$
\begin{equation*}
c^{*}(\boldsymbol{\Phi})=\min _{\mathbf{W}, \mathbf{H}} c(\mathbf{\Phi}, \mathbf{W}, \mathbf{H})=\sum_{m n}\left(1+\log \mathbb{E}\left([\boldsymbol{\Phi} \mathbf{Y}]_{m n}^{2}\right)\right) \tag{12}
\end{equation*}
$$

and that this minimal value is attained at any point $(\mathbf{W}, \mathbf{H})$ that verifies $\mathbf{W H}=\mathbb{E}\left(|\boldsymbol{\Phi} \mathbf{Y}|^{\circ}\right.$ ). To prove (12), it is sufficient to show that, under conditions (5)-(6), there exists an exact NMF of $\mathbb{E}\left(|\boldsymbol{\Phi} \mathbf{Y}|^{\circ 2}\right)$ for any $\boldsymbol{\Phi}$. Let $\mathbf{D}=\boldsymbol{\Phi} \overline{\boldsymbol{\Phi}}^{\top}$, so that $\boldsymbol{\Phi}=$ $\mathbf{D} \overline{\mathbf{\Phi}}$. Denote $\overline{\mathbf{V}}=\overline{\mathbf{W}} \overline{\mathbf{H}}, \bar{v}_{m n}=[\overline{\mathbf{V}}]_{m n}$ and $d_{m m^{\prime}}=[\mathbf{D}]_{m m^{\prime}}$. From (5) and (6) we have

$$
\begin{align*}
\mathbb{E}\left([\mathbf{\Phi} \mathbf{Y}]_{m n}^{2}\right) & =\mathbb{E}\left(\left(\sum_{m^{\prime}} d_{m m^{\prime}}[\overline{\mathbf{\Phi}} \mathbf{Y}]_{m^{\prime} n}\right)^{2}\right)  \tag{13}\\
& =\sum_{m^{\prime}} d_{m m^{\prime}}^{2} \bar{v}_{m^{\prime} n} \tag{14}
\end{align*}
$$

Hence, because all the terms in (14) are non-negative and the rank of the matrix $\overline{\mathbf{V}}$ is at most $\bar{K} \leq K$, we have derived an exact NMF of $\mathbb{E}\left(|\boldsymbol{\Phi} Y|^{\circ 2}\right)$ which proves (12). As $\boldsymbol{\Phi}$ is orthogonal, one can verify that the objective $c^{*}(\boldsymbol{\Phi})$ is equivalent to the one used in [12], [14].

Then, it follows that

$$
\begin{equation*}
c^{*}(\boldsymbol{\Phi})=\sum_{m n} \log \left(\left[\left(\boldsymbol{\Phi} \overline{\boldsymbol{\Phi}}^{\mathbf{\top}}\right)^{\circ 2} \overline{\mathbf{V}}\right]_{m n}\right)+N M \tag{15}
\end{equation*}
$$

It remains to prove that $\min _{\boldsymbol{\Phi}} c^{*}(\boldsymbol{\Phi})$ is attained at $\boldsymbol{\Phi}=\overline{\boldsymbol{\Phi}}$. Using the fact that $\mathbf{D}=\boldsymbol{\Phi} \bar{\Phi}^{\top}$ is orthogonal and thus that both the columns and the rows of $\mathbf{D}^{\circ 2}$ sum to one, we obtain from Jensen's inequality

$$
\begin{equation*}
\log \left(\sum_{m^{\prime}} d_{m m^{\prime}}^{2} \bar{v}_{m^{\prime} n}\right) \geq \sum_{m^{\prime}} d_{m m^{\prime}}^{2} \log \left(\bar{v}_{m^{\prime} n}\right) \tag{16}
\end{equation*}
$$

This implies the following lower bound on $c^{*}(\boldsymbol{\Phi})$

$$
\begin{align*}
c^{*}(\boldsymbol{\Phi}) & \geq \sum_{m n} \sum_{m^{\prime}} d_{m m^{\prime}}^{2} \log \left(\bar{v}_{m^{\prime} n}\right)+N M  \tag{17}\\
& =\sum_{m^{\prime} n} \log \left(\bar{v}_{m^{\prime} n}\right)+N M=c^{*}(\overline{\mathbf{\Phi}}) \tag{18}
\end{align*}
$$

Moreover, one can see that $c^{*}(\overline{\mathbf{\Phi}})=c\left(\overline{\mathbf{\Phi}}, \mathbf{W}^{\star}, \mathbf{H}^{\star}\right)$ for any $\mathbf{W}^{\star} \in \mathbb{R}_{+}^{M \times K}$ and $\mathbf{H}^{\star} \in \mathbb{R}_{+}^{K \times N}$ such that $\mathbf{W}^{\star} \mathbf{H}^{\star}=\overline{\mathbf{V}}=$ $\mathbb{E}\left(|\overline{\mathbf{\Phi}} \mathbf{Y}|^{\circ 2}\right.$ ) (using (14) and the fact that for $\left.\boldsymbol{\Phi}=\overline{\boldsymbol{\Phi}}, \mathbf{D}=\mathbf{I}\right)$. This completes the proof.

## B. Proof of Theorem 1

Let $(\boldsymbol{\Phi}, \mathbf{W}, \mathbf{H})$ be a global minimizer of $c$ such that $c(\boldsymbol{\Phi}, \mathbf{W}, \mathbf{H})=c^{*}(\overline{\boldsymbol{\Phi}})$. Following the results in Lemma 1, we are going to show that $\forall q \in\{1, \ldots, Q\}$, there exists a partition $\left\{B_{q}\right\}_{q=1}^{Q}$ of $\{1, \ldots, M\}$ such that $\boldsymbol{\operatorname { s p a n }}_{B_{q}}(\boldsymbol{\Phi})=\operatorname{span}_{\bar{B}_{q}}(\overline{\boldsymbol{\Phi}})$. By definition of $\bar{B}_{q}$, we denote $\hat{v}_{q n}=\bar{v}_{m n}$ for $m \in \bar{B}_{q}$. Hence $\forall q^{\prime} \neq q$, there exists $n \in\{1, \ldots, N\}$ such that $\hat{v}_{q n} \neq \hat{v}_{q^{\prime} n}$. As $c(\mathbf{\Phi}, \mathbf{W}, \mathbf{H})=c^{*}(\overline{\mathbf{\Phi}})$, the equality holds in (16) and we can write it as

$$
\begin{equation*}
\forall n, \quad \log \left(\sum_{q=1}^{Q} \hat{d}_{m q}^{2} \hat{v}_{q n}\right)=\sum_{q=1}^{Q} \hat{d}_{m q}^{2} \log \left(\hat{v}_{q n}\right) \tag{19}
\end{equation*}
$$

where $\hat{d}_{m q}^{2}=\sum_{m^{\prime} \in \bar{B}_{q}} d_{m m^{\prime}}^{2}$. We will show at the end of the proof that $\forall m \in\{1, \ldots, M\}$ there exists $\tau(m) \in\{1, \ldots, Q\}$ such that

$$
\hat{d}_{m q}^{2}= \begin{cases}1 & \text { if } q=\tau(m)  \tag{20}\\ 0 & \text { if } q \neq \tau(m)\end{cases}
$$

From (20), we can construct $B_{q}=\{m: \tau(m)=q, 1 \leq m \leq$ $M\}$ so that

$$
\begin{equation*}
\hat{d}_{m q}^{2}=\sum_{m^{\prime} \in \bar{B}_{q}} d_{m m^{\prime}}^{2}=1 \quad \text { if } \quad m \in B_{q} \tag{21}
\end{equation*}
$$

By the definition of $d_{m m^{\prime}}$ and the orthogonality of $\boldsymbol{\Phi}$ and $\overline{\boldsymbol{\Phi}}$, (21) implies that each row of $\boldsymbol{\Phi}$ in the set $B_{q}$ belongs to $\boldsymbol{\operatorname { s p a n }}_{\bar{B}_{q}}(\overline{\boldsymbol{\Phi}})$. Therefore $\boldsymbol{\operatorname { s p a n }}_{B_{q}}(\boldsymbol{\Phi}) \subset \operatorname{span}_{\bar{B}_{q}}(\bar{\Phi})$.

To show that $\boldsymbol{\operatorname { s p a n }}_{B_{q}}(\boldsymbol{\Phi})=\operatorname{span}_{\bar{B}_{q}}(\overline{\boldsymbol{\Phi}})$, we first check that

$$
\begin{equation*}
\forall q, \quad\left|B_{q}\right|=\sum_{m=1}^{M} \hat{d}_{m q}^{2}=\sum_{m^{\prime} \in \bar{B}_{q}} \sum_{m=1}^{M} d_{m m^{\prime}}^{2}=\left|\bar{B}_{q}\right| \tag{22}
\end{equation*}
$$

From (22), we also obtain a similar formula as (21)

$$
\begin{equation*}
\sum_{m \in B_{q}} d_{m m^{\prime}}^{2}=1 \quad \text { if } \quad m^{\prime} \in \bar{B}_{q} \tag{23}
\end{equation*}
$$

Therefore $\boldsymbol{\operatorname { s p a n }}_{\bar{B}_{q}}(\overline{\boldsymbol{\Phi}}) \subset \operatorname{span}_{B_{q}}(\boldsymbol{\Phi})$.
Finally we show that (20) is correct by absurd. Assume that (20) is not true. Hence there exist $m$ and $q^{\prime} \neq q$, such that

$$
\begin{equation*}
\hat{d}_{m q}^{2} \in(0,1) \text { and } \hat{d}_{m q^{\prime}}^{2} \in(0,1) \tag{24}
\end{equation*}
$$

Then, the fact that $\sum_{q} \hat{d}_{m q}^{2}=\sum_{m^{\prime}} d_{m m^{\prime}}^{2}=1$ together with the strict concavity of the $\log$ function imply that the equality (19) can hold only if $\hat{v}_{q n}=\hat{v}_{q^{\prime} n}, \forall n$. This contradicts the fact that $\bar{B}_{q} \cap \bar{B}_{q^{\prime}}=\emptyset$ and completes the proof.

