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

$$c^*(\mathbf{\Phi}) = \min_{\mathbf{W},\mathbf{H}} c(\mathbf{\Phi}, \mathbf{W}, \mathbf{H}) = \sum_{mn} (1 + \log \mathbb{E}([\mathbf{\Phi}\mathbf{Y}]_{mn}^2)), \ (12)$$

and that this minimal value is attained at any point (\mathbf{W}, \mathbf{H}) that verifies $\mathbf{W}\mathbf{H} = \mathbb{E}(|\mathbf{\Phi}\mathbf{Y}|^{\circ 2})$. To prove (12), it is sufficient to show that, under conditions (5)–(6), there exists an exact NMF of $\mathbb{E}(|\mathbf{\Phi}\mathbf{Y}|^{\circ 2})$ for any $\mathbf{\Phi}$. Let $\mathbf{D} = \mathbf{\Phi}\bar{\mathbf{\Phi}}^{\mathsf{T}}$, so that $\mathbf{\Phi} =$ $\mathbf{D}\bar{\mathbf{\Phi}}$. Denote $\bar{\mathbf{V}} = \bar{\mathbf{W}}\bar{\mathbf{H}}$, $\bar{v}_{mn} = [\bar{\mathbf{V}}]_{mn}$ and $d_{mm'} = [\mathbf{D}]_{mm'}$. From (5) and (6) we have

$$\mathbb{E}([\mathbf{\Phi}\mathbf{Y}]_{mn}^2) = \mathbb{E}\left(\left(\sum_{m'} d_{mm'} [\bar{\mathbf{\Phi}}\mathbf{Y}]_{m'n}\right)^2\right)$$
(13)

$$=\sum_{m'} d_{mm'}^2 \bar{v}_{m'n}.$$
 (14)

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

Then, it follows that

$$c^*(\mathbf{\Phi}) = \sum_{mn} \log([(\mathbf{\Phi}\bar{\mathbf{\Phi}}^{\mathsf{T}})^{\circ 2}\bar{\mathbf{V}}]_{mn}) + NM.$$
(15)

It remains to prove that $\min_{\Phi} c^*(\Phi)$ is attained at $\Phi = \Phi$. Using the fact that $\mathbf{D} = \Phi \overline{\Phi}^{\mathsf{T}}$ 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

$$\log\left(\sum_{m'} d_{mm'}^2 \bar{v}_{m'n}\right) \ge \sum_{m'} d_{mm'}^2 \log(\bar{v}_{m'n}).$$
(16)

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

$$c^{*}(\mathbf{\Phi}) \geq \sum_{mn} \sum_{m'} d_{mm'}^{2} \log(\bar{v}_{m'n}) + NM$$
(17)
= $\sum \log(\bar{v}_{m'n}) + NM = c^{*}(\bar{\mathbf{\Phi}}).$ (18)

$$= \sum_{m'n} \log(\bar{v}_{m'n}) + NM = c^*(\bar{\Phi}).$$
(18)

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

B. Proof of Theorem 1

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

$$\forall n, \quad \log\left(\sum_{q=1}^{Q} \hat{d}_{mq}^2 \hat{v}_{qn}\right) = \sum_{q=1}^{Q} \hat{d}_{mq}^2 \log(\hat{v}_{qn}), \quad (19)$$

where $\hat{d}_{mq}^2 = \sum_{m' \in \bar{B}_q} d_{mm'}^2$. 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

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

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

$$\hat{d}_{mq}^2 = \sum_{m' \in \bar{B}_q} d_{mm'}^2 = 1 \quad \text{if} \quad m \in B_q.$$
 (21)

By the definition of $d_{mm'}$ and the orthogonality of Φ and $\bar{\Phi}$, (21) implies that each row of Φ in the set B_q belongs to $\operatorname{span}_{\bar{B}_q}(\bar{\Phi})$. Therefore $\operatorname{span}_{B_q}(\Phi) \subset \operatorname{span}_{\bar{B}_q}(\bar{\Phi})$.

To show that $\operatorname{span}_{B_a}(\Phi) = \operatorname{span}_{\bar{B}_a}(\bar{\Phi})$, we first check that

$$\forall q, \quad |B_q| = \sum_{m=1}^M \hat{d}_{mq}^2 = \sum_{m' \in \bar{B}_q} \sum_{m=1}^M d_{mm'}^2 = |\bar{B}_q|.$$
 (22)

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

$$\sum_{m \in B_q} d_{mm'}^2 = 1 \quad \text{if} \quad m' \in \bar{B}_q.$$
⁽²³⁾

Therefore $\operatorname{span}_{\bar{B}_a}(\Phi) \subset \operatorname{span}_{B_a}(\Phi)$.

Finally we show that (20) is correct by absurd. Assume that (20) is not true. Hence there exist m and $q' \neq q$, such that

$$\hat{d}_{mq}^2 \in (0,1) \text{ and } \hat{d}_{mq'}^2 \in (0,1).$$
 (24)

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