Robustness Analysis of HottTopixx, a Linear Programming Model for Factoring Nonnegative Matrices

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Abstract

Although nonnegative matrix factorization (NMF) is NP-hard in general, it has been shown very recently that it is tractable under the assumption that the input nonnegative data matrix is separable (that is, there exists a cone spanned by a small subset of the columns containing all columns). Since then, several algorithms have been designed to handle this subclass of NMF problems. In particular, Bittorf, Recht, Ré and Tropp ('Factoring nonnegative matrices with linear programs', NIPS 2012) proposed a linear programming model, referred to as HottTopixx. In this paper, we provide a new and more general robustness analysis of their method. In particular, our analysis is almost tight and allows duplicates and near duplicates in the dataset. Moreover, we design a provably more robust variant using an appropriate post-processing strategy.

Keywords. Nonnegative matrix factorization, separability, robustness, linear programming, HottTopixx.

1 Introduction

Nonnegative matrix factorization (NMF) is a popular machine learning technique and allows to express a set of nonnegative vectors as nonnegative linear combinations of nonnegative basis elements [9]. More formally, given a nonnegative matrix $M \in \mathbb{R}^{m\times n}_+$ corresponding to n vectors in an m-dimensional space and a factorization rank r, the aim is to find a basis matrix $U \in \mathbb{R}^{m\times r}_+$ and a weight matrix $V \in \mathbb{R}^{r\times n}_+$ such that the norm of the error $M - UV$ is minimized. Although NMF is NP-hard [10], Arora et al. [1] recently showed that it can be solved in polynomial time given that the matrix M is separable. A nonnegative matrix $M \in \mathbb{R}^{m\times n}_+$ is r-separable if and only if it can be expressed as $M = WH$, where $W \in \mathbb{R}^{m\times r}_+$, $H \in \mathbb{R}^{r\times n}_+$, and each column of W is equal to a column of M. In other terms, $M \in \mathbb{R}^{m\times n}_+$ is r-separable if and only if

$$M \;=\; W\,[I_r, H']\Pi \;=\; [W, WH']\Pi,$$

for some $H' \in \mathbb{R}^{r\times n}_+$ and some permutation matrix $\Pi \in \{0,1\}^{n\times n}$. Any nonnegative matrix is n-separable because of the trivial decomposition $M = MI$ with $r = n$, and the aim is to find a decomposition where r is as small as possible. It is rather straightforward to check that the smallest such r is the number of extreme rays of the cone generated by the columns of M, that is, $\text{cone}(M) = \{Mx \mid x \in \mathbb{R}^n_+\}$. Equivalently, if the columns of matrix M are normalized to sum to one, the smallest such r is the number of vertices of the convex hull of the columns of M, that is, $\text{conv}(M) = \{Mx \mid x \in \mathbb{R}^n_+, \sum_{i=1}^n x_i = 1\}$; see [8] and the references therein for more details about the geometric interpretation of the separable NMF problem.

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It turns out that the separability assumption makes sense in several practical situations. For example, in document classification, each column of M corresponds to a document (that is, a vector of word counts) and is approximated with a nonnegative linear combination of the columns of matrix W which correspond to different topics (that is, bags of words). Separability of M requires that, for each topic, there exists at least one document discussing only that topic. Separability of M^T (that is, each row of H appears as a row of M) requires that, for each topic, there exists at least one word used only by that topic; see [1, 2] and the references therein. The separability assumption is also widely used in hyperspectral imaging and is referred to as the pure-pixel assumption, see [7] and the references therein.

In practice, the input separable matrix M is perturbed with some noise and it is therefore desirable to design robust algorithms; see [1, 2, 3, 5, 6, 7, 8]. In this paper, we will focus on the algorithm of Bittorf, Recht, Ré and Tropp [3], referred to as HottTopixx, which is described in the next section. As we will see, the robustness result provided by the authors is rather restrictive as it does not allow near duplicates in the dataset: the aim of this paper is to develop a more general analysis of their algorithm.

1.1 HottTopixx: a Linear Programming Model for Separable NMF

From now on, we will *always* assume that the columns of the input data matrix M have been normalized in order to sum to one, that is,

(i) The zero columns of M have been discarded, and

(ii) Each column of M is updated using $M(:,j) \leftarrow \frac{M(:,j)}{||M(:,j)||_1}$.

We will also always assume that we are given a noisy separable matrix $\tilde{M} = M + N$ where $N \in \mathbb{R}^{m \times n}$ is some noise added to the separable matrix M such that

$$||N||_1 = \max_{||x||_1 \leq 1} ||Nx||_1 = \max_j ||N(:,j)||_1 \leq \epsilon, \quad \text{for some } \epsilon \geq 0.$$

The matrix M is r-separable if and only if

$$M = WH = W[I_r, H']\Pi = [W, WH']\Pi = [W, WH'] \underbrace{\begin{pmatrix} I_r & H' \\ 0_{(n-r)\times r} & 0_{(n-r)\times(n-r)} \end{pmatrix} \Pi}_{X \in \mathbb{R}^{n \times n}_+} = MX, \tag{1}$$

for some $H' \geq 0$ and some permutation matrix Π. Equation (1) shows that M is r-separable if and only if there exists a nonnegative matrix $X \in \mathbb{R}^{n \times n}_+$ such that : (1) X contains $(n-r)$ all-zero rows and the r-by-r identity matrix as a submatrix (up to permutation), and (2) $M = MX$. Notice that because the columns of matrix M and W sum to one, the columns of the matrix H' have sum to one as well. Based on this observation, Bittorf et al. [3] proposed to solve the following optimization problem[1] in order to identifying approximately the columns of the matrix W among the columns of the matrix $\tilde{M}$:

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times n}_+} \quad & p^T \operatorname{diag}(X) \\ \text{such that} \quad & ||\tilde{M} - \tilde{M}X||_1 \leq 2\epsilon, \\ & \operatorname{tr}(X) = r, \\ & X(i,i) \leq 1 \text{ for all } i, \\ & X(i,j) \leq X(i,i) \text{ for all } i, j, \end{aligned} \tag{2}$$

[1]In [3], the model assumes separability of M^T so that (2) is equivalent to the model in [3] applied to M^T. We prefer here to work with the columns.

where $p \in \mathbb{R}^n$ is any vector with distinct entries. Intuitively, the model reads as follows: we have to assign a weight to each column of M (that is, give a value to $X(i,i)$ for all i) for a total weight of r. Moreover, we cannot use a column to reconstruct another column with a weight larger than the corresponding diagonal entry of X, while we have to guarantee that the approximation error is small. It is interesting to notice that the problem is always feasible: in fact,

$$X^0 = \begin{pmatrix} I_r & H' \\ 0_{(n-r)\times r} & 0_{(n-r)\times(n-r)} \end{pmatrix} \Pi, \quad \text{with } M = MX^0,$$

is a feasible solution of (2) since the columns of H' sum to one and

$$\begin{aligned} ||\tilde{M} - \tilde{M}X^0||_1 &= ||(M+N) - (M+N)X^0||_1 \\ &\leq ||M - MX^0||_1 + ||N||_1 + ||NX^0||_1 \leq 2\epsilon. \end{aligned}$$

Finally, Bittorf et al. [3] proposed Algorithm 1 to identifying approximately the columns of W among the columns of $\tilde{M}$, while the corresponding optimal weight matrix H can be obtained by solving another linear program, see Algorithm 2.

Algorithm 1 HottTopixx - Extracting Columns of a Separable Matrix by Linear Programming [3]

Input: A noisy r-separable matrix $\tilde{M} = WH + N$, where $||N||_1 \leq \epsilon$ and W is α-robustly simplicial.
Output: A matrix $\tilde{W}$ such that $||\tilde{W}(:,P) - W||_1 \leq \delta$ for some permutation P and some $\delta \geq 0$.

1: Find the optimal solution X^* of (2).
2: Let $\mathcal{K}$ be the index set corresponding to the r largest diagonal entries of X^*.
3: Set $\tilde{W} = \tilde{M}(:,\mathcal{K})$.

Algorithm 2 Approximably Separable NMF using HottTopixx and Linear Programming [3]

Input: A noisy r-separable matrix $\tilde{M} = WH + N$, where $||N||_1 \leq \epsilon$ and W is α-robustly simplicial.
Output: An nonnegative factorization $(\tilde{W}, \tilde{H})$ such that $||\tilde{M} - \tilde{W}\tilde{H}||_1 \leq \epsilon + \delta$.

1: Compute $\tilde{W}$ using Algorithm 1.
2: Solve $\tilde{H} = \operatorname{argmin}_{Y \geq 0} ||\tilde{M} - \tilde{W}Y||_1$.

Before stating robustness results, it is important to define the conditioning of matrix W, which is a crucial characteristic of separable NMF problems. In fact, the better the columns of W are spread in the unit simplex $\Delta^m = \{x \in \mathbb{R}^m \mid x \geq 0, \sum_{i=1}^m = 1\}$, the more noise tolerant the data will be. In [1, 3], this conditioning is measured via the following parameter:

$$\alpha = \min_{1 \leq k \leq r, x \in \Delta^{r-1}} ||W(:,k) - W(:,\mathcal{R})x||_1, \quad \text{where } \mathcal{R} = \{1,2,\dots,r\} \backslash \{k\},$$

and the matrix W is said to be *α-robustly simplicial.* (Notice that $\alpha \leq 2$ for any nonnegative matrix W whose columns sum to one.) In other words, α is the minimum among the ℓ_1-distances between a column of W and the convex hull of the other columns of W. It is necessary that $||N||_1 \leq \epsilon < \frac{\alpha}{2}$ for *any* separable NMF algorithm to be able to approximately recover the columns of W from the matrix $\tilde{M} = WH + N$. In fact, if $\epsilon \geq \frac{\alpha}{2}$, any r-separable matrix M with $r \geq 2$ can be perturbed so that one of the columns of the perturbed matrix $\tilde{M}$ corresponding to a column of W belongs to the convex hull of the other columns. In other words, we can perturb the matrix M so that it becomes $(r-1)$-separable and we could therefore not distinguish one of the columns of W from the columns of M. For example, with

$$W = \begin{pmatrix} \frac{\alpha}{2} I_r \\ (1 - \frac{\alpha}{2})e^T \end{pmatrix}, H = I_r \text{ and } N = \begin{pmatrix} \frac{-\alpha}{2} I_r \\ 0 \end{pmatrix}, \text{ we have } \tilde{M} = \begin{pmatrix} 0_{r\times r} \\ (1 - \frac{\alpha}{2})e^T \end{pmatrix},$$

so that the matrix $M = WH$ is r-separable while $\tilde{M}$ is 1-separable.

In order to prove robustness results for Algorithm 2, Bittorf et al. [3] used the following observation:

Lemma 1. *Suppose M is normalized and admits a rank-r separable factorization WH, and suppose $\tilde{M} = M + N$ with $||N||_1 \leq \epsilon$. If $\tilde{W}$ is such that $||\tilde{W}(:,P) - W||_1 \leq \delta$ for some $\delta \geq 0$ and some permutation P, then Algorithm 2 constructs a factorization $(\tilde{W}, \tilde{H})$ satisfying $||\tilde{M} - \tilde{W}\tilde{H}||_1 \leq \epsilon + \delta$.*

Proof. Denoting $N_W = \tilde{W}(:,P) - W$, we have

$$
\begin{aligned}
||\tilde{M} - \tilde{W}\tilde{H}||_1 &= \operatorname{argmin}_{Y \geq 0} ||M + N - (W + N_W)Y||_1 \\
&\leq ||M + N - (W + N_W)H||_1 \\
&\leq ||N||_1 + ||N_W H||_1 + ||M - WH||_1 \\
&\leq \epsilon + \delta,
\end{aligned}
$$

since the columns of H sum to one. $\square$

Lemma 1 allows us to focusing on proving robustness results for Algorithm 1. In fact, any result that applies to Algorithm 1 directly applies to Algorithm 2. In this paper, we will therefore focus our attention on Algorithm 1, as it was implicitly done in [3, 4].

In the first version of their paper [4], two different robustness results were proposed. The first one assumes that there is no duplicates or near-duplicate of the columns of W in the dataset, which amounts for the maximum entry of H' in Equation (1) to be bounded above:

Proposition 1. *Suppose $\tilde{M} = M + N$ where M is normalized, admits a rank-r separable factorization WH with W α-robustly simplicial and $||N||_1 \leq \epsilon$, and has the form (1) with[2] $||H'||_\infty = \max_{i,j} |H'_{ij}| \leq \beta \leq 1$. Suppose $\epsilon \leq f(\alpha, \beta, r)$ for some function f. Then Algorithm 1 extracts a matrix $\tilde{W}$ satisfying $||W - \tilde{W}(:,P)||_1 \leq \epsilon$ for some permutation P.*

The second one is general as it does not make any assumption on matrix H':

Proposition 2. *Suppose $\tilde{M} = M + N$ where M is normalized, and admits a rank-r separable factorization WH with W α-robustly simplicial and $||N||_1 \leq \epsilon$. Suppose $\epsilon \leq g(\alpha, r)$ for some function g. Then Algorithm 1 extracts a matrix $\tilde{W}$ satisfying $||W - \tilde{W}(:,P)||_1 \leq \delta$ for some permutation P and some $\delta \geq 0$.*

The aim is to finding functions f and g as large as possible and δ as small as possible such that the propositions above hold. In [4, Prop. 3.3] (resp. [4, Prop. 3.2]) authors originally claimed that $f(\alpha, \beta, r) = \frac{1}{2}\alpha(1-\beta)$ (resp. $g(\alpha, r) = \frac{\alpha^2}{8+4\alpha}$ and $\delta = 4\epsilon$) gives the result. Unfortunately, there were some flaws in the proofs, as is shown by the following counter example. Let

$$
W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, H = \begin{pmatrix} 1 & 0 & 0 & 1/3 \\ 0 & 1 & 0 & 1/3 \\ 0 & 0 & 1 & 1/3 \end{pmatrix} = M,
$$

$N = 0$ and $\epsilon = 0.15$ so that $\tilde{M} = M = WH$ with

$$
\beta = \frac{1}{3}, \quad \alpha = 2, \quad \text{and} \quad ||N||_1 = 0 \leq \epsilon = 0.15 \leq \frac{\alpha^2}{8 + 4\alpha} = 0.25 \leq \frac{1}{2}\alpha(1-\beta) = \frac{2}{3},
$$

hence the conditions of [4, Prop. 3.2] and [4, Prop. 3.3] are satisfied. However,

$$
X^* = \begin{pmatrix} 0.7 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0 \\ 0 & 0 & 0.7 & 0 \\ 0 & 0 & 0 & 0.9 \end{pmatrix}
$$

[2] Usually $||A||_p = \max_{||x||_p \leq 1} ||Ax||_p$ hence $||A||_\infty$ should refer to $\max_i ||A(i,:)||_1$ but we assign it a different meaning in this paper.

is an optimal solution of (2) with $p = (1, 2, 3, -1)^T$, so that the last column of $\tilde{M}$ is selected by Algorithm 1, which gives

$$||\tilde{W}(:, P) - W||_1 = 2 > 4\epsilon = 0.6 \quad \text{ and } \quad \min_{H \geq 0} ||\tilde{M} - \tilde{W}H||_1 = 1 > 4\epsilon,$$

for any permutation P, a contradiction with Propositions 3.2 and 3.3 in [4].

In the final version [3], only the following robustness result is proposed :

Proposition 3 ([3], Prop. 3.2). *Suppose $\tilde{M} = M + N$ where M is normalized, and admits a rank-r separable factorization WH with W α-robustly simplicial and $||N||_1 \leq \epsilon$. Suppose for each column $M(:, j)$ $1 \leq j \leq n$ either $M(:, j) = W(:, k)$ for some $1 \leq k \leq r$ or $||M(:, j) - W(:, k)||_1 \geq d_0$ for all $1 \leq k \leq r$. If $\epsilon < \frac{\alpha d_0}{8r}$ and $d_0 \leq \frac{\alpha}{2}$, then Algorithm 1 extracts a matrix $\tilde{W}$ satisfying* $\min_{H \geq 0} ||\tilde{M} - \tilde{W}H||_1 \leq 2\epsilon$.

By Lemma 1 and the fact that (see Lemma 4)

$$||M(:, j) - W(:, k)||_1 > d_0 \text{ for all } 1 \leq k \leq r \quad \Rightarrow \quad ||H(:, j)||_\infty < \beta = 1 - \frac{d_0}{2},$$

Proposition 3 is essentially equivalent to Proposition 1. The only differences are that (1) Proposition 3 allows duplicates of the columns of W in the dataset, and (2) Proposition 1 does not need any assumption[3] on β.

Finally, the robustness result proposed in [3] only deals with input data matrices without near duplicates. In this paper, we propose a variant of HottTopixx (Algorithm 3) which is more robust, and applies to any separable matrix.

1.2 Conditioning and κ-Robustly Conical Matrices

Because the columns of the variable X in (2) are not required to sum to one (note that this constraint could be added to the model while keeping linearity), it turns out that it will be easier to work with the following parameter measuring the conditioning of matrix W:

$$\kappa = \min_{1 \leq k \leq r} \min_{x \in \mathbb{R}^{r-1}_+} ||W(:, k) - W(:, \mathcal{R})x||_1, \quad \text{ where } \mathcal{R} = \{1, 2, \dots, r\} \backslash \{k\},$$

and the matrix W is said to be *κ-robustly conical.* We have that κ is the minimum among the ℓ_1-distances between a column of W and the convex *cone* generated by the other columns of W. If the columns of W sum to one (which will always be assumed), $\kappa \leq 1$ and we can relate α and κ as follows:

Theorem 1. *For any α-robustly simplicial and κ-robustly conical nonnegative matrix W whose columns sum to one, we have*

$$\kappa \quad \leq \quad \alpha \quad \leq \quad 2\kappa.$$

Proof. The first inequality follows directly from the definition. The second is proved in Appendix A. □

Therefore, it is essentially equivalent to working with α or κ as they differ by a multiplicative factor of at most 2.

[3] At the time we write this paper, the proof of Proposition 3 is not publicly available, and it is not clear why the condition $d_0 \leq \frac{\alpha}{2}$ is needed. In fact, it seems that Proposition 3 contradicts Theorem 4: a more natural condition on d_0 would be a lower bound, such as $d_0 \geq \frac{\alpha}{2}$ (which would be rather restrictive as one of the columns of W is at distance α of the convex hull of the other columns of W).

1.3 Contribution and Outline of the Paper

In this paper, we provide a new robustness analysis of Algorithm 1. In Section 2, we focus on Proposition 1 and prove that

- $\epsilon \leq \frac{\kappa(1-\beta)}{7(r+1)}$ is sufficient for Proposition 1 to hold (Theorem 2), while
- $\epsilon < \frac{\kappa(1-\beta)}{(1-\beta)(r-1)+1}$ is necessary for Proposition 1 to hold for any $r \geq 3$ and $\beta < 1$ (Theorem 3).

This shows that our analysis is close to being tight. Moreover, the second condition on ϵ implies that it is necessary for Proposition 2 to hold that $\epsilon < \frac{\kappa}{r-1}$ (Corollary 1). In Section 3, we focus on Proposition 2 and first show that it is necessary that $\delta \geq 3\frac{\epsilon}{\alpha} + \frac{3}{2}\epsilon$ for any $\epsilon < \frac{\alpha}{2}$ (Theorem 4). (We also show that this lower bound on δ applies to a broader class of separable NMF algorithms.) Then, we propose a post-processing of the solution of the linear program (2) (see Algorithm 3) for which the following result holds:

(Theorem 5) *Let $M = WH$ be a normalized r-separable matrix with W κ-robustly conical. Let also $\tilde{M} = M + N$ with $||N||_1 \leq \epsilon$. If*

$$\epsilon < \frac{\omega\kappa}{74(r+1)},$$

where $\omega = \min_{i\neq j} ||W(:,i) - W(:,j)||_1$, then Algorithm 3 extracts a matrix $\tilde{W}$ such that

$$||W - \tilde{W}(:,P)||_1 \leq 37(r+1)\frac{\epsilon}{\kappa} + 2\epsilon, \quad \textit{for some permutation } P.$$

Because the necessary condition $\epsilon < \frac{\kappa}{r-1}$ also applies to Algorithm 3, the bound for ϵ of Theorem 5 is tight up to a factor ω (and some constant multiplicative factor). Moreover, because of Theorem 4, the bound for δ of Theorem 5 is tight up to a factor r (and some constant multiplicative factor). Finally, we show that it is necessary for Proposition 2 to hold that $\epsilon \leq \frac{\kappa}{(r-1)^2}$ for any $\delta < \kappa + \epsilon$ (Theorem 6) which demonstrates that HottTopixx cannot achieve a better bound than Algorithm 3.

1.4 Notation

The set of m-by-n real matrices is denoted $\mathbb{R}^{m\times n}$; for $A \in \mathbb{R}^{m\times n}$, we denote the jth column of A by $A(:,j)$, the ith row of A by $A(i,:)$, and the entry at position (i,j) by $A(i,j)$; for $b \in \mathbb{R}^{m\times 1} = \mathbb{R}^m$, we denote the ith entry of b by $b(i)$. Notation $A(\mathcal{I},\mathcal{J})$ refers to the submatrix of A with row and column indices respectively in $\mathcal{I}$ and $\mathcal{J}$. The matrix A^T is the transpose of A. The ℓ_1-norm $||.||_1$ of a vector is defined as $||b||_1 = \sum_i |b(i)|$ and of a matrix as $||A||_1 = \max_j ||A(:,j)||_1$. We will denote by E_n the n-by-n matrix of all-ones, $0_{m\times n}$ the m-by-n the matrix of all-zeros, and I_n the n-by-n identity matrix. We will also denote e_i the ith column of the identity matrix, e the all-one vector and 0 the all-zero vector; their dimensions will be clear from the context. The vector of the diagonal entries of a matrix A is denoted $\mathrm{diag}(A)$ while its trace is denoted $\mathrm{tr}(A) = e^T \mathrm{diag}(A)$. For a set $\mathcal{K}$, $|\mathcal{K}|$ denotes its cardinality.

2 Analysis of Proposition 1

In this section, we show that $\epsilon \leq \frac{\kappa(1-\beta)}{7(r+1)}$ is sufficient for Proposition 1 to hold (Theorem 2), while $\epsilon < \frac{\kappa(1-\beta)}{(r+1)(1-\beta)+1}$ is necessary for any $r \geq 3$ and $\beta < 1$ (Theorem 3).

Lemma 2. *Suppose $\tilde{M} = M + N$ where M is normalized and $||N||_1 \leq \epsilon < 1$, and suppose X is a feasible solution of (2). Then, for all $1 \leq j \leq n$,*

$$||X(:,j)||_1 \leq 1 + \frac{2\epsilon}{1-\epsilon} \quad \textit{and} \quad ||M(:,j) - MX(:,j)||_1 \leq 2\epsilon\left(\frac{2-\epsilon}{1-\epsilon}\right).$$

Proof. For all $1 \le j \le n$, $||\tilde{M}(:,j) - \tilde{M}X(:,j)||_1 \le 2\epsilon$ so that

$$1-\epsilon \le ||M(:,j)||_1 - ||N(:,j)||_1 \le ||M(:,j)+N(:,j)||_1 = ||\tilde{M}(:,j)||_1 \le ||M(:,j)||_1 + ||N(:,j)||_1 \le 1+\epsilon.$$

We then have

$$\begin{aligned} 2\epsilon \ge ||\tilde{M}(:,j) - \tilde{M}X(:,j)||_1 &\ge ||\tilde{M}X(:,j)||_1 - ||\tilde{M}(:,j)||_1 \\ &\ge ||\tilde{M}X(:,j)||_1 - ||\tilde{M}||_1 \\ &\ge ||\tilde{M}||_1(||X(:,j)||_1 - 1) \\ &\ge (1-\epsilon)(||X(:,j)||_1 - 1), \end{aligned}$$

hence $||X(:,j)||_1 \le 1 + \frac{2\epsilon}{1-\epsilon}$ implying that $||NX(:,j)||_1 \le ||N||_1 ||X(:,j)||_1 \le \epsilon\left(1 + \frac{2\epsilon}{1-\epsilon}\right)$. Therefore,

$$\begin{aligned} 2\epsilon \ge ||\tilde{M}(:,j) - \tilde{M}X(:,j)||_1 &= ||M(:,j) + N(:,j) - (M+N)X(:,j)||_1 \\ &\ge ||M(:,j) - MX(:,j)||_1 - \epsilon - \epsilon\left(1 + \frac{2\epsilon}{1-\epsilon}\right), \end{aligned}$$

from which we obtain $||M(:,j) - MX(:,j)||_1 \le 2\epsilon\left(2 + \frac{\epsilon}{1-\epsilon}\right) = 2\epsilon\left(\frac{2-\epsilon}{1-\epsilon}\right)$. □

Lemma 3. *Let $\tilde{M} = M + N$ where M is normalized, admits a rank-r separable factorization WH with W κ-robustly conical and $||N||_1 \le \epsilon$, and has the form (1) with $||H'||_\infty = \max_{i,j} |H'_{ij}| \le \beta < 1$. Let also X be any feasible solution of (2), then*

$$X(j,j) \ge 1 - \frac{2\epsilon}{\kappa(1-\beta)}\left(\frac{3-\epsilon}{1-\epsilon}\right) \qquad \textit{for all } j \textit{ such that } M(:,j) = W(:,k) \textit{ for some } 1 \le k \le r\ .$$

Proof. Let $\mathcal{K}$ be the set of r indices such that $M(:,\mathcal{K}) = W$. Let also $1 \le k \le r$ and denote $j = \mathcal{K}(k)$ so that $M(:,j) = W(:,k)$. By Lemma 2,

$$||W(:,k) - WHX(:,j)||_1 \le 2\epsilon\left(\frac{2-\epsilon}{1-\epsilon}\right). \tag{3}$$

Since $H(k,j) = 1$,

$$\begin{aligned} WHX(:,j) &= W(:,k)H(k,:)X(:,j) + W(:,\mathcal{R})H(\mathcal{R},:)X(:,j) \\ &= W(:,k)\Big(X(j,j) + H(k,\mathcal{J})X(\mathcal{J},j)\Big) + W(:,\mathcal{R})y, \end{aligned}$$

where $\mathcal{R} = \{1,2,\dots,r\}\backslash\{k\}$, $\mathcal{J} = \{1,2,\dots,n\}\backslash\{j\}$ and $y = H(\mathcal{R},:)X(:,j) \ge 0$. We have

$$\eta = X(j,j) + H(k,\mathcal{J})X(\mathcal{J},j) \le X(j,j) + \beta\left(1 + \frac{2\epsilon}{1-\epsilon} - X(j,j)\right), \tag{4}$$

since $||H(k,\mathcal{J})||_\infty \le \beta$ and $||X(:,j)||_1 \le 1 + \frac{2\epsilon}{1-\epsilon}$ (Lemma 2). Hence

$$||W(:,k) - WHX(:,j)||_1 \ge (1-\eta)\left|\left|W(:,k) - W(:,\mathcal{R})\frac{y}{1-\eta}\right|\right|_1 \ge (1-\eta)\kappa. \tag{5}$$

Combining Equations (3), (4) and (5), we obtain

$$1 - \left(X(j,j) + \beta\left(1 + \frac{2\epsilon}{1-\epsilon} - X(j,j)\right)\right) \le \frac{2\epsilon}{\kappa}\left(\frac{2-\epsilon}{1-\epsilon}\right),$$

which gives, using the fact that $(\kappa\beta)^{-1} \ge 1$,

$$X(j,j) \ge 1 - \frac{2\epsilon}{\kappa(1-\beta)}\left(\frac{3-\epsilon}{1-\epsilon}\right).$$

□

Theorem 2. *It is sufficient for Proposition 1 to hold that*

$$\epsilon \leq \frac{\kappa(1-\beta)}{7(r+1)}.$$

Proof. If $\epsilon = 0$, the proof is given in [3, Prop. 3.1]: for each $1 \leq k \leq r$, there exists $1 \leq j \leq n$ such that $M(:,j) = W(:,k)$ and $X(j,j) = 1$ (this follows easily from the fact that the entries of p are distinct). Otherwise $\epsilon > 0$ and $\beta < 1$. Let X be a feasible solution of (2) (which always exists since the feasible set of (2) is non-empty). If we prove that the r diagonal entries of X corresponding to the columns of W are larger than all the other ones (because $\beta < 1$, the are no duplicates of the columns of W in the dataset), then we are done. In fact, these columns will then be identified by Algorithm 2 and we will have $||W - \tilde{W}(:,P)||_1 \leq \epsilon$ for some permutation P. (Notice that we do not need an optimal solution: any feasible solution identifies the columns of W.)

Let $\mathcal{K}$ be the set of r indices such that $M(:,\mathcal{K}) = W$. Assume that

$$X(k,k) > \frac{r}{r+1} \qquad \text{for all } k \in \mathcal{K}. \tag{6}$$

Since $\mathrm{tr}(X) = r$ and $X \geq 0$, we have

$$\sum_{j \notin \mathcal{K}} X(j,j) = r - \sum_{k \in \mathcal{K}} X(k,k) < r - r\frac{r}{r+1} = \frac{r}{r+1} < X(k,k) \quad \text{ for all } k \in \mathcal{K},$$

implying that $X(j,j) < X(k,k)$ for all $k \in \mathcal{K}, j \notin \mathcal{K}$ which gives the result. It remains to show that (6) holds. By Lemma 3,

$$X(k,k) \geq 1 - \frac{2\epsilon}{\kappa(1-\beta)}\left(\frac{3-\epsilon}{1-\epsilon}\right) > 1 - \frac{7\epsilon}{\kappa(1-\beta)},$$

since $\frac{3-\epsilon}{1-\epsilon} < 3.5$ for any $\epsilon \leq \frac{\kappa(1-\beta)}{7(r+1)} \leq \frac{1}{14}$ as $0 \leq \kappa, \beta \leq 1$ and $r \geq 1$. Finally, for $\epsilon \leq \frac{(1-\beta)\kappa}{7(r+1)}$, $X(i,i) > \frac{r}{r+1}$ and the proof is complete. □

Remark 1. *The proof of Theorem 2 actually does not make use of the constraints $X(i,j) \leq X(i,i)$. The reason is that the assumption $||H'||_\infty \leq \beta < 1$ implies that there is no duplicate of the columns of W in the dataset (if $\beta = 1$, $\epsilon = 0$ and Algorithm 2 is guaranteed to work [3, Prop. 3.1]). This implies that for being able to reconstruct sufficiently well each column of W, the corresponding diagonal entry of X must be large independently of the other entries of the corresponding column of X.*

Therefore, in case we know there is no duplicate in the dataset (or have used some pre-processing to remove them), these constraints can be discarded (a similar observation was made in [3, 4]). Moreover, since Theorem 2 only requires feasibility in that case, any feasible solution of the corresponding relaxed linear program will correctly identify the columns of W.

Theorem 3. *For Proposition 1 to hold when $r \geq 3$ and $\beta < 1$, it is necessary that*

$$\epsilon < \frac{\kappa(1-\beta)}{(r-1)(1-\beta)+1}. \tag{7}$$

Proof. See Appendix B. □

Theorem 3 shows that the sufficient condition derived in Theorem 2 is close to being tight. In particular, if r is assumed to be bounded above, then it is tight up to some constant multiplicative factor (in practice r is often assumed to be small). We believe it is possible to improve the bound of Theorem 2 to match the one of Theorem 3 (up to some constant multiplicative factor). Unfortunately, we were not able to derive such a sufficient condition; this is a topic for further research.

Corollary 1. *For Proposition 2 to hold for any $\delta < \frac{\kappa}{2}$ and $r \geq 3$, it is necessary that*

$$\epsilon < \frac{\kappa}{r-1},$$

Proof. In fact,

$$\epsilon < \frac{\kappa(1-\beta)}{(1-\beta)(r-1)+1} \leq \frac{\kappa(1-\beta)}{(1-\beta)(r-1)} = \frac{\kappa}{r-1},$$

while the matrix $\tilde{M} = WH + N$ constructed in the proof of Theorem 3 satisfies $||W - \tilde{W}(:,P)||_1 \geq \frac{r-2}{r-1}\kappa \geq \frac{\kappa}{2}$ where $\tilde{W}$ is the matrix extracted by Algorithm 1 and P is any permutation. □

Remark 2 (Cases $r = 1, 2$)**.** *Theorem 3 does not apply when $r = 1, 2$ because:*

- *The rank-one separable NMF problem is trivial. In fact, if M admits a rank-one separable factorization wh^T and $\tilde{M} = M + N$ with $||N||_1 \leq \epsilon$, then $||\tilde{M}(:,j) - w||_1 \leq \epsilon$ for all j.*
- *The rank-two case is particular because it is not possible to construct very bad instances. In fact, all rank-two separable NMF problems are essentially equivalent to each other because the columns of M belong to the line segment $[W(:,1), W(:,2)]$.*

3 Analysis of Proposition 2 and Post-Processing Strategy

In this section, we investigate Proposition 2 and propose a variant of HottTopixx (see Algorithm 3) which is more robust and applicable to any noisy separable matrix. In Section 3.1, we present a simple necessary condition for Proposition 2 to hold. In Section 3.2, we show that, for each column of W, there is a subset of the columns of $\tilde{M}$ close to that column of W such that the sum of the corresponding diagonal entries of any feasible solution X of (2) is larger than $\frac{r}{r+1}$. Therefore, using an appropriate post-processing of the solution X of (2) (see Algorithm 3), we can approximately recover the columns of W, given that the noise level ϵ is smaller than some upper bound. Finally, we show in Section 3.3 that HottTopixx (Algorithm 1) cannot achieve this bound which shows that Algorithm 3 is more robust.

3.1 Preliminary Necessary Conditions

Recall the aim is to identifying, among the columns of $\tilde{M}$, r columns gathered in the matrix $\tilde{W}$ such that $||W - \tilde{W}(:,P)||_1 \leq \delta$ for some permutation P and some $\delta \geq 0$. Since $||W||_1 = 1$, we will assume that $\delta < 1$ otherwise the separable NMF problem is trivial since the solution $\tilde{W} = 0$ gives the result. It actually makes sense to impose $\delta < \kappa \leq \alpha \leq 1$: this guarantees for a solution $\tilde{W}$ to have distinct columns since two columns of W can potentially be at distance κ; for example with

$$W = \begin{pmatrix} \frac{\kappa}{2} & 0 \\ 0 & \frac{\kappa}{2} \\ 1-\frac{\kappa}{2} & 1-\frac{\kappa}{2} \end{pmatrix},$$

extracting twice the first column would give the result with $\delta = \kappa$, which is not desirable. Moreover, as shown in Section 1.1, it is necessary that $\epsilon < \frac{\alpha}{2} \leq \kappa$ for *any* separable NMF algorithm to being able to extract approximately the columns of W.

Theorem 4. *For any $0 \leq \epsilon < \frac{\alpha}{2}$, it is necessary that $\delta \geq \left(3\frac{\epsilon}{\alpha} + \frac{3}{2}\epsilon\right)$ for Proposition 2 to hold.*

Proof. Let us consider $\tilde{M} = M + N = WH + N$ where

$$W = \begin{pmatrix} 1 & 0 & \frac{1}{2}-\frac{\alpha}{4} \\ 0 & 1 & \frac{1}{2}-\frac{\alpha}{4} \\ 0 & 0 & \frac{\alpha}{2} \end{pmatrix}, H = \begin{pmatrix} 1 & 0 & 0 & 1-\lambda & 0 \\ 0 & 1 & 0 & 0 & 1-\lambda \\ 0 & 0 & 1 & \lambda & \lambda \end{pmatrix}, \text{ and } N = \begin{pmatrix} 0 & 0 & \frac{\epsilon}{4} & 0 & 0 \\ 0 & 0 & \frac{\epsilon}{4} & 0 & 0 \\ 0 & 0 & -\frac{\epsilon}{2} & 0 & 0 \end{pmatrix},$$

where W is α-robustly simplicial (and $\frac{\alpha}{2}$-robustly conical), and where λ is such that the middle point between $M(:,4)$ and $M(:,5)$ is $\left(\tilde{M}(:,3) + 2N(:,3)\right)$, that is,

$$\tilde{M}(:,3) + 2N(:,3) = \begin{pmatrix} \frac{1}{2} - \frac{\alpha}{4} + \frac{3\epsilon}{4} \\ \frac{1}{2} - \frac{\alpha}{4} + \frac{3\epsilon}{4} \\ \frac{\alpha}{2} - \frac{3\epsilon}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} - \frac{\lambda\alpha}{4} \\ \frac{1}{2} - \frac{\lambda\alpha}{4} \\ \frac{\lambda\alpha}{2} \end{pmatrix} = \frac{1}{2}(M(:,4) + M(:,5)),$$

which requires $\lambda = 1 - 3\frac{\epsilon}{\alpha} \geq 0$. Let $p = (-K, -K, K^2, -1, 0)^T$ for any K sufficiently large. It can be checked that

$$X = \begin{pmatrix} 1 & 0 & 0 & \mu & 0 \\ 0 & 1 & 0 & 0 & \mu \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 & 0.5 - \mu \\ 0 & 0 & 0.5 & 0.5 - \mu & 0.5 \end{pmatrix} \qquad \text{where } \mu = \frac{1-\lambda}{2-\lambda},$$

is a feasible solution of (2). By Lemma 7, there exists K sufficiently large such that $X^*(3,3) = 0$ for any optimal solution X^*. Using Lemma 7 again we have $X^*(1,1) = X^*(2,2) = 1$ for any optimal solution X^* for K sufficiently large. Hence, for K sufficiently large, the third column of M will not be extracted and the fourth or fifth will be, hence

$$\begin{aligned} ||\tilde{W} - W||_1 = ||\tilde{W}(:,3) - W(:,3)||_1 &= ||M(:,4) - W(:,3)||_1 = ||M(:,5) - W(:,3)||_1 \\ &= ||(1-\lambda)W(:,1) - (1-\lambda)W(:,3)||_1 \\ &= 3\frac{\epsilon}{\alpha} \|W(:,1) - W(:,3)\|_1 \\ &= 3\frac{\epsilon}{\alpha}\left(1 + \frac{\alpha}{2}\right) = 3\frac{\epsilon}{\alpha} + \frac{3}{2}\epsilon. \end{aligned}$$

□

Using the same construction[4] as in Theorem 4 but taking $\lambda = 1 - \frac{\epsilon}{\alpha}$, we have

$$\tilde{M}(:,3) = W(:,3) + N(:,3) = \frac{1}{2}\left(M(:,4) + M(:,5)\right),$$

for which $||\tilde{W}(:,P) - W||_1 \geq \frac{\epsilon}{\alpha} + \frac{\epsilon}{2}$ for any permutation P, where $\tilde{W}$ is the matrix extracted by HottTopixx. We notice that the corresponding matrix $\tilde{M}$ can also be obtained from a 4-separable matrix $M_4 = W_4 H_4$ where

$$W_4 = \begin{pmatrix} M(:,[1\,2]) & M(:,4) - v & M(:,5) - v \end{pmatrix}, H_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 1 & 0 \\ 0 & 0 & 0.5 & 0 & 1 \end{pmatrix},$$

$v = (\epsilon/4, \epsilon/4, -\epsilon/2)^T$, and

$$N_4 = \begin{pmatrix} 0_{3\times 2} & v & v & v \end{pmatrix},$$

and we have $\tilde{M} = WH + N = W_4H_4 + N_4 = \tilde{M}_4$. Therefore,

> *No algorithm to which only the noisy separable matrix $\tilde{M}$ and the noise level ϵ are given as input can approximately extract the columns of W among the columns of M with error smaller than $\mathcal{O}\left(\frac{\epsilon}{\alpha}\right)$.*

[4] A Matlab code is available at `https://sites.google.com/site/nicolasgillis/code` containing this construction, along with the one of Theorem 4.

In fact, the matrix $\tilde{M}$ above has two solutions to the noisy separable NMF problem and there is no way to discriminate between them (the original matrix could be 3- or 4- separable):

- If the algorithm returns a matrix $\tilde{W}$ with three columns, then if the original matrix was M_4 we have $\max_{1\leq j\leq 4}\min_{1\leq k\leq 3}||W_4(:,j)-\tilde{W}(:,k)||_1 \geq \frac{\epsilon}{\alpha}$.
- Similarly, if the algorithm returns a matrix $\tilde{W}$ with four columns, then
  - if the third column is not extracted and the original matrix was M, we have

$$\max_{1\leq j\leq 3}\min_{1\leq k\leq 4}||W(:,j)-\tilde{W}(:,k)||_1 \geq \frac{\epsilon}{\alpha}, \quad \text{while}$$

  - if the third column is extracted and the original matrix was M_4, we have

$$\max_{1\leq j\leq 4}\min_{1\leq k\leq 4}||W_4(:,j)-\tilde{W}(:,k)||_1 \geq \frac{\epsilon}{\alpha}.$$

The reason is that the distance between each pair of columns of M is at least $\frac{\epsilon}{\alpha}$.

Note that the algorithm of Arora et al. [1] achieves this optimal bound $\mathcal{O}\left(\frac{\epsilon}{\alpha}\right)$. However, it requires the parameter α as an input so that the construction above does not prove their algorithm is optimal up to some constant multiplicative factor. In fact, for the 3-separable matrix M, W is α-robustly simplicial while, for the 4-separable matrix M_4, W_4 is α'-robustly simplicial with $\alpha' \leq 2\frac{\epsilon}{\alpha} = ||W_4(:,3)-W_4(:,4)||_1$.

3.2 Cluster Identification

We now prove that there is a cluster of columns of $\tilde{M}$ around each column of W for which the sum of the corresponding diagonal entries of any feasible solution X of (2) is large. More formally, defining the clusters around the columns of W as

$$\Omega_k^\rho = \left\{ j \;\middle|\; ||\tilde{M}(:,j)-W(:,k)||_1 \leq \rho \right\} \quad 1\leq k\leq r, \tag{8}$$

we are going to prove that $c_k = \sum_{j\in\Omega_k^\rho} X(j,j)$ is large for any feasible solution X of (2), given that ϵ is sufficiently small.

Lemma 4. *Let $W \in \mathbb{R}_+^{m\times r}$ have its columns sum to one, and let $h \in \Delta^m$. Then, denoting $k = \operatorname{argmax}_{1\leq i\leq r} h(i)$, we have*

$$||h||_\infty = h(k) \geq 1-\frac{\rho}{2} \quad \Rightarrow \quad ||W(:,k)-Wh||_1 \leq \rho.$$

Proof. Let us denote denote $\mathcal{R} = \{1,2,\dots,r\}\backslash\{k\}$, we have

$$\begin{aligned} ||W(:,k)-Wh||_1 &= ||(1-h(k))W(:,k)-W(:,K)h(\mathcal{R})||_1 \\ &\leq (1-h(k))||W(:,k)||_1 + (||h||_1-h_k)||W(:,\mathcal{R})||_1 \\ &\leq 2(1-h(k)) \leq \rho. \end{aligned}$$

□

Lemma 5. *Let $M = WH$ be a normalized r-separable matrix with W κ-robustly conical. Let also $\tilde{M} = M+N$ where $||N||_1 \leq \epsilon < 1$, and X be a feasible solution of (2). Then, the total weight $c_k = \sum_{j\in\Omega_k^\rho} X(j,j)$ assigned to the columns of $\tilde{M}$ in Ω_k^ρ defined in (8) satisfies*

$$c_k \geq 1-\frac{4\epsilon}{\kappa\rho}\left(\frac{3-\epsilon}{1-\epsilon}\right) \qquad \textit{for all } 1\leq k\leq r.$$

Proof. Let $1 \leq k \leq r$ and $\mathcal{R} = \{1, 2, \dots, r\} \backslash \{k\}$, and let us denote the indices corresponding to the columns of $\tilde{M}$ not in Ω_k^ρ as

$$\bar{\Omega}_k^\rho = \{1, 2, \dots, n\} \backslash \Omega_k^\rho.$$

Let also j be such that $W(:,k) = M(:,j)$. By Lemma 4, $||H(:, \bar{\Omega}_k^\rho)||_\infty < 1 - \frac{\rho}{2} = \beta$. The rest of the proof is similar to that of Lemma 3. By Lemma 2, $||W(:,k) - WHX(:,j)||_1 \leq 2\epsilon \left(\frac{2-\epsilon}{1-\epsilon}\right)$ and $||X(:,j)||_1 \leq 1 + \frac{2\epsilon}{1-\epsilon}$. We have

$$\begin{aligned} WHX(:,j) &= W(:,k)H(k,:)X(:,j) + W(:,\mathcal{R})H(\mathcal{R},:)X(:,j) \\ &= W(:,k)\Big(H(k,\Omega_k^\rho)X(\Omega_k^\rho, j) + H(k, \bar{\Omega}_k^\rho)X(\bar{\Omega}_k^\rho, j)\Big) + W(:,\mathcal{R})y, \end{aligned}$$

where $y = H(\mathcal{R},:)X(:,j) \geq 0$, and

$$\begin{aligned} \eta &= H(k,\Omega_k^\rho)X(\Omega_k^\rho, j) + H(k, \bar{\Omega}_i^\rho)X(\bar{\Omega}_i^\rho, j) \\ &\leq ||X(\Omega_k^\rho, j)||_1 + \beta(||X(:,j)||_1 - ||X(\Omega_k^\rho, j)||_1) \leq c_k + \beta \left(1 + \frac{2\epsilon}{1-\epsilon} - c_k\right). \end{aligned}$$

The first inequality follows from $H(i,j) \leq 1$ for all i,j and $||H(k, \bar{\Omega}_k^\rho)||_\infty \leq \beta$; the second from $X(i,j) \leq X(i,i)$ for all i,j (hence $c_k \geq ||X(\Omega_k^\rho, j)||_1$), and $\beta \leq 1$. Finally, $(1-\eta)\kappa \leq ||W(:,k) - WHX(:,j)||_1 \leq 2\epsilon \left(\frac{2-\epsilon}{1-\epsilon}\right)$ leading to $c_k = \sum_{j \in \Omega_k^\rho} X(j,j) \geq 1 - \frac{2\epsilon}{\kappa(1-\beta)} \left(\frac{3-\epsilon}{1-\epsilon}\right) = 1 - \frac{4\epsilon}{\kappa\rho} \left(\frac{3-\epsilon}{1-\epsilon}\right)$. □

If we can guarantee that $c_k > \frac{r}{r+1}$ for all $1 \leq k \leq r$, then the sum of the diagonal entries of X corresponding to columns of $\tilde{M}$ not in any Ω_k^ρ will be smaller than $\frac{r}{r+1}$. Therefore, if instead of picking the r largest diagonal entries of X, we cluster the diagonal entries of X depending on the distances between the corresponding columns of $\tilde{M}$, we should be able to identifying the columns of W approximately; see Algorithm 3.

Algorithm 3 Extracting Columns of a Separable Matrix by Linear Programming and Clustering

Input: A r-separable matrix $\tilde{M} = WH + N$ with $||N||_1 \leq \epsilon < \frac{\kappa\omega}{74(r+1)}$ and W is κ-robustly conical.

Output: A matrix $\tilde{W}$ such that $||\tilde{W}(:,P) - W||_1 \leq 37(r+1)\frac{\epsilon}{\kappa} + 2\epsilon$ for some permutation P.

Compute the optimal solution X of (2).
Initialize $\mathcal{K} = \{k \mid X(k,k) > \frac{r}{r+1}\}$ and $\nu = 2\epsilon$.
while $|\mathcal{K}| < r$ **do**
    Compute $\mathcal{K}$ with Algorithm 4 using input $m_j = \tilde{M}(:,j)$ $1 \leq j \leq n$, $x = \text{diag}(X)$ and ν;
    $\nu \leftarrow 2\nu$;
end while
$\tilde{W} = \tilde{M}(:,\mathcal{K})$;

Lemma 6. *Let $m_j \in \mathbb{R}^m$ $1 \leq j \leq n$, $x \in \mathbb{R}_+^n$ be such that $\sum_{j=1}^n x = r$, and $\rho \geq 0$. Let also $\Omega_k = \{m_j \mid ||m_j - w_k||_1 \leq \rho\}$ for $1 \leq k \leq r$ where $w_k \in \mathbb{R}^m$ $1 \leq k \leq r$. Suppose*

- $\sum_{j \in \Omega_k} x_j > \frac{r}{r+1}$,
- $\omega = \min_{i \neq j} ||w_i - w_j||_1 > 6\rho$, *and*
- *For all $1 \leq k \leq r$, there exists $1 \leq j \leq n$ such that $||m_j - w_k||_1 \leq \epsilon \leq \rho$.*

Then, for any $(\rho + \epsilon) \leq \nu \leq 2(\rho + \epsilon)$, Algorithm 4 identifies a set $\mathcal{K}$ with r indices such that

$$\max_{1 \leq k \leq r} \min_{j \in \mathcal{K}} ||m_j - w_k||_1 \leq 3\rho + 2\epsilon. \tag{9}$$

Moreover, if Algorithm 4 identifies a set $\mathcal{K}$ with r indices for some $\nu < \rho + \epsilon$, then $\mathcal{K}$ satisfies (9).

Algorithm 4 Cluster Extraction

Input: A set of points m_j $1 \leq j \leq n$, a vector of weights $x \in \mathbb{R}^n_+$ such that $\sum_{i=j}^n x = r$, and $\nu \geq 0$.
Output: A index set $\mathcal{K}$ of centroids corresponding to clusters with weight strictly larger than $\frac{r}{r+1}$.

```
D(i,j) = ||m_i - m_j||_1 for 1 ≤ i,j ≤ n.
S_i = {j | D(i,j) ≤ ν} for 1 ≤ i ≤ n;
w(i) = Σ_{j∈S_i} x(j) for 1 ≤ i ≤ n;
K = ∅;
while max_{1≤i≤n} w(i) > r/(r+1) do
    k = argmax w(i);
    K ← K ∪ {k};
    For all j ∈ S_k : w(j) ← 0;
    For all i ∉ S_k and j ∈ S_k such that j ∈ S_i : w(i) ← w(i) − x(j);
end while
```

Proof. First notice that the index set $\mathcal{K}$ extracted by Algorithm 4 cannot contain more than r indices. In fact, Algorithm 4 only identifies clusters with weight strictly larger than $\frac{r}{r+1}$ while the total weight $\sum_{i=1}^n x$ is equal to r. It remains to show that $\mathcal{K}$ contains at least r indices.

Let first consider the case $(\rho + \epsilon) \leq \nu \leq 2(\rho + \epsilon)$. Let $\mathcal{S}_i$ $1 \leq i \leq n$ be the sets computed by Algorithm 4 before entering the while loop. We observe that

- For $m_j \in \Omega_k$ and $m_{j'} \in \Omega_{k'}$ where $j \neq j'$ and $k \neq k'$, we have $m_j \notin \mathcal{S}_{j'}$ and $m_{j'} \notin \mathcal{S}_j$. In fact,

$$||m_j - m_{j'}||_1 = ||(m_i - w_k) + (w_k - w_{k'}) + (w_{k'} - m_{j'})||_1 \geq \omega - 2\rho > 4\rho \geq \nu.$$

- For all $1 \leq k \leq r$, there exists $m_j \in \Omega_k$ such that $w(j) > \frac{r}{r+1}$. By assumption, for all $1 \leq k \leq r$, there exists $m_j \in \Omega_k$ such that $||m_j - w_k||_1 \leq \epsilon$, hence for all $m_i \in \Omega_k$ we have $||m_j - m_i||_1 = ||(m_j - w_k) + (w_k - m_i)||_1 \leq \rho + \epsilon \leq \nu$ while $\sum_{i \in \Omega_k} x(i) > \frac{r}{r+1}$.

- If $m_i \notin \cup_{1 \leq k \leq r} \Omega_k$ and $w(i) > \frac{r}{r+1}$, then $||m_i - w_k||_1 \leq 3\rho + 2\epsilon$ for some $1 \leq k \leq r$. Suppose $||m_i - w_k||_1 > 3\rho + 2\epsilon$ for all k, then

$$||m_i - m_j||_1 \geq ||(m_i - w_k) + (w_k - m_j)||_1 > 3\rho + 2\epsilon - \rho \geq \nu \quad \text{for all } m_j \in \cup_{1 \leq k \leq r} \Omega_k.$$

  Therefore, $\sum_{j \in \mathcal{S}_i} x(j) \leq r - \sum_k \sum_{j \in \Omega_k} x_i < r - r\frac{r}{r+1} < \frac{r}{r+1}$, a contradiction.

  Let then k be such that $||m_i - w_k||_1 \leq 3\rho + 2\epsilon$. This implies that if $m_j \in \mathcal{S}_i$, then either $m_j \in \Omega_k$, or $m_j \notin \cup_{k' \neq k} \Omega_{k'}$. In fact, if $m_j \in \Omega_{k'}$ for some $k' \neq k$, then

$$||m_i - m_j||_1 \geq ||(m_i - w_k) + (w_k - w_{k'}) + (w_{k'} - m_j)||_1 \geq \omega - 3\rho - 2\epsilon - \rho > 2\rho - 2\epsilon \geq \nu,$$

  a contradiction.

These observations imply that there are at least r disjoint sets $\mathcal{S}_i$ with weight larger than $\frac{r}{r+1}$, each corresponding to a different cluster Ω_k. Therefore, Algorithm 4 will identify them individually and (9) will be satisfied.

For the case $\nu < \rho + \epsilon$, the result follows directly from the observations above: any point m_i with $w(i) > \frac{r}{r+1}$ must satisfy $||m_i - w_k||_1 \leq 3\rho + 2\epsilon$ for some $1 \leq k \leq r$. Moreover, for all k there must exist $j \in \mathcal{K}$ such that $||m_j - w_k||_1 \leq 3\rho + 2\epsilon$. In fact, suppose there exists k such that $||m_j - w_k|| > 3\rho + 2\epsilon$ for all $j \in \mathcal{K}$. Then, $m_i \notin \cup_{j \in \mathcal{K}} \mathcal{S}_j$ for all $i \in \Omega_k$ (see above) hence $\sum_{i \in \mathcal{S}_j, j \in \mathcal{K}} x(i) < r - \frac{r}{r+1} = r\frac{r}{r+1}$ which implies that $\mathcal{K}$ cannot contain more than $r - 1$ indices, a contradiction. $\square$

Theorem 5. *Let $M = WH$ be a normalized r-separable matrix with W κ-robustly conical. Let also $\tilde{M} = M + N$ with $||N||_1 \leq \epsilon$. If*

$$\epsilon < \frac{\omega\kappa}{74(r+1)},$$

where $\omega = \min_{i \neq j} ||W(:,i) - W(:,j)||_1$, then Algorithm 3 will extract a matrix $\tilde{W}$ such that

$$||W - \tilde{W}(:,P)||_1 \leq \delta = 37(r+1)\frac{\epsilon}{\kappa} + 2\epsilon, \qquad \textit{for some permutation } P.$$

Proof. Let X be a feasible solution of (2), let the r clusters Ω_k^ρ $1 \leq k \leq r$ be defined as in Equation (8) and let $c_k = \sum_{j \in \Omega_k^\rho} X(j,j)$. If $\rho < \frac{\omega}{6}$ and $c_k > \frac{r}{r+1}$, then, by Lemma 6, Algorithm 4 will identify a set $\mathcal{K}$ with r indices such that

$$\max_{1 \leq k \leq r} \min_{j \in \mathcal{K}} ||W(:,k) - \tilde{M}(:,j)||_1 \leq \delta = 3\rho + 2\epsilon,$$

for any $\nu \in [\rho + \epsilon, 2\rho + 2\epsilon]$. Therefore, starting with $\nu = 2\epsilon \leq (\rho + \epsilon)$ and multiplying it by two at each iteration will eventually give a value of ν in $[\rho + \epsilon, 2\rho + 2\epsilon]$. (Note that Algorithm 4 could return a set $\mathcal{K}$ with r indices for ν smaller than $\rho + \epsilon$, see Lemma 6. Note also that the number of iterations performed by Algorithm 3 is at most $\log_2\left(\frac{\rho+\epsilon}{\epsilon}\right)$.) If $\epsilon = 0$, then $c_k = 1$ for all $1 \leq k \leq r$ while $\rho = 0 < \frac{\omega}{6}$, and the loop is entered at most once (if the entries of p are distinct, then it is not entered because exactly r diagonal entries of an optimal solution of (2) will be equal to one, each corresponding to a different column of W [3, Prop. 3.1]). Otherwise $\epsilon > 0$ and it remains to guarantee that $\rho < \frac{\omega}{6}$ and $c_k > \frac{r}{r+1}$. By Lemma 5,

$$\epsilon\left(\frac{3-\epsilon}{1-\epsilon}\right) < \frac{\rho\kappa}{4(r+1)} \quad \Rightarrow \quad c_k > \frac{r}{r+1}.$$

Taking $\epsilon < \frac{\omega\kappa}{74(r+1)}$ and $\rho = \frac{37}{3}(r+1)\frac{\epsilon}{\kappa} < \frac{\omega}{6}$ completes the proof since

$$\rho = \frac{37}{3}(r+1)\frac{\epsilon}{\kappa} > 4(r+1)\frac{\epsilon}{\kappa}\left(\frac{3-\epsilon}{1-\epsilon}\right),$$

because $3 \leq \frac{3-\epsilon}{1-\epsilon} < \frac{37}{12}$ for any $0 \leq \epsilon < 10^{-2}$ (as $74(r+1) \geq 100$ for $r \geq 1$). $\square$

It can be checked that all the results from Section 2 apply to Algorithm 3. In fact, by assumption, all the matrices considered did not contain duplicate or near-duplicate of the columns of matrix W. In fact, we showed that r diagonal entries of X have weight at least $\frac{r}{r+1}$ implying that Algorithm 3 will not enter the while loop, hence it is equivalent to Algorithm 1. In particular, Corollary 1 also applies to Algorithm 3, that is, it is necessary that

$$\epsilon < \frac{\kappa}{r-1}, \qquad \text{for any } \delta < \frac{\kappa}{2}.$$

This shows that the bound of Theorem 5 for ϵ is tight up to a factor ω (and some constant multiplicative factor). Moreover, by Theorem 4, the bound for δ is tight up to a factor r (and some constant multiplicative factor).

Remark 3 (Computational Cost). *The main additional cost of Algorithm 3 compared to Algorithm 1 is to computing and storing the distance matrix D. This requires $\mathcal{O}(mn^2)$ floating point operations and $\mathcal{O}(n^2)$ space in memory. This is negligible as computing MX already requires $\mathcal{O}(mn^2)$ operations, while storing X requires $\mathcal{O}(n^2)$ space in memory. Notice that if $\operatorname{diag}(X)$ contains zero entries, they can be discarded along with the corresponding data points.*

Remark 4 (Choice of the vector p). *Because of the post-processing procedure in Algorithm 3, it is not necessary for Theorem 5 to hold that the vector p has distinct entries. However, it will still be useful in practice to impose this condition. In fact, this will incite the weights to be concentrated in fewer diagonal entries of X so that typically fewer loops will have to be performed to obtain a set $\mathcal{K}$ containing r indices. In particular, in the exact case (that is, $\epsilon = 0$) or in the case there is no duplicate and near duplicate in the dataset (see above), the loop will not be entered.*

Remark 5 (More Sophisticated Post-processing Strategies). *It is possible to design better post-processing procedures but we wanted here to keep the analysis simple. In particular, if the input matrix $\tilde{M}$ does not satisfy the conditions of Theorem 5, it may happen that no set $\mathcal{K}$ computed in the loop of Algorithm 3 contains r elements. Therefore, one should keep in memory the largest set extracted so far, or design more sophisticated strategies. For example, if less than r clusters have been extracted, the condition that the weight of each extracted cluster must larger than $\frac{r}{r+1}$ can be relaxed; this variant has been implemented in the Matlab code available at `https://sites.google.com/site/nicolasgillis/code`.*

3.3 Repartition of the Weights inside a Cluster

In this last section, we show that HottTopixx (Algorithm 1) cannot provide better bounds than Algorithm 3. The reason is the following: inside a cluster Ω_k^ρ, there is no guarantee that all the weight will be assigned to a single diagonal entry of X (as originally claimed in [4]). In the proof of Theorem 6, we show that the weight may be equally distributed inside a cluster. This construction allows us to show that $\epsilon \leq \frac{\kappa}{(r-1)^2}$ is necessary for Proportion 2 to hold for any $\delta < \kappa + \epsilon$, which proves our claim.

Theorem 6. *For any $r \geq 3$ and $\delta < \kappa + \epsilon$, it is necessary for Proposition 2 to hold that*

$$\epsilon \leq \frac{\kappa}{(r-1)^2}.$$

Proof. See Appendix C. □

A Matlab code is available at `https://sites.google.com/site/nicolasgillis/code` containing the constructions from Theorems 3, 4 and 6, and the post-processing procedure (Algorithm 3). In particular, the construction from Theorem 6 provides examples where Algorithm 3 is more robust than HottTopixx.

4 Conclusion and Further Work

In this paper, we proposed a more robust variant of HottTopixx based on an appropriate post-processing of the solution of the linear program (2) (see Algorithm 3). We proved that Algorithm 3 is robust for any input separable matrix M (Theorem 5), while our analysis is close to being tight.

It would be interesting to improve the bound of Theorem 5 or show that the bound is tight. It would also be particularly interesting to design more robust or computationally more effective (or both?) separable NMF algorithms.

Appendix A. Proof of Theorem 1

Proof of Theorem 1. Let

$$k = \operatorname{argmin}_{1 \leq j \leq r} \min_{x \in \mathbb{R}^{r-1}_+} ||W(:,j) - W(:,\mathcal{J})x||_1, \quad \text{where } \mathcal{J} = \{1,2,\dots,r\} \backslash \{j\},$$

$w = W(:,k)$, and

$$y = \text{argmin}_{x \in \mathbb{R}^{r-1}_+} ||W(:,k) - W(:,\mathcal{R})x||_1, \quad \text{ where } \mathcal{R} = \{1,2,\dots,r\}\backslash\{k\},$$

so that, by definition, $||y - w||_1 = \kappa$. If $y = 0$, we are done since $\kappa = ||w||_1 = 1 \geq \frac{1}{2}\alpha$ as $\alpha \leq 2$. Otherwise $y \neq 0$ and we define $z = \frac{y}{||y||_1} = \lambda^{-1}y$. By definition, $||w - z||_1 \geq \alpha$ since z belongs to the convex hull of the columns of W. We have

$$\alpha \leq ||w - z||_1 = ||w - (\lambda + 1 - \lambda)z||_1 \leq ||w - \lambda z||_1 + (1-\lambda)||z||_1 = \kappa + (1-\lambda) \leq 2\kappa$$

since $\kappa = ||w - \lambda z||_1 \geq ||w||_1 - ||\lambda z||_1 = 1 - \lambda$, and the proof is complete. □

Appendix B. Proof of Theorem 3

The following lemma shows that if one of the coefficients in the objective function of a linear program is much larger than all the other ones, then the corresponding entry of any optimal solution must be smaller than the corresponding entry of any feasible solution. Although the result is clear intuitively, we provide here a simple proof.

Lemma 7. *Let consider the following linear program*

$$\min_{x \in \mathbb{R}^n} c_K^T x \quad \text{ such that } \; Ax = b \; \text{ and } \; l \leq x \leq u, \tag{10}$$

with $l, u \in \mathbb{R}^n$, $l \leq u$, and $c_K = (K, \tilde{c}) \in \mathbb{R}^n$ where $K \in \mathbb{R}$ is a parameter. Let us denote x_K^* an optimal solution of (10) *depending on K. Assume there exists a feasible solution x^f of* (10) *such that $x^f(1) = s$. Then, for any K sufficiently large, $x_K^*(1) \leq s$.*

Similarly, if $c_K(1) = -K$ and there exists a feasible solution such that $x(1) = t$, Then, for any K sufficiently large, $x_K^*(1) \geq t$.

Proof. Let $\mathcal{V} \neq \emptyset$ be the set of vertices of the feasible set of (10), and $\bar{\mathcal{V}} = \{x \in \mathcal{V} \mid x(1) > s\}$. Notice that because the feasible set of (10) is a polytope, there always exists an optimal solution in $\mathcal{V}$. Let us denote $d = \min_{x \in \bar{\mathcal{V}}} x(1) > s$. Assume there exists an optimal solution x_K^* such that $x_K^*(1) > s$. This implies that there exists an optimal solution $\bar{x}_K^* \in \bar{\mathcal{V}}$ (since any optimal solution is a convex combination of optimal vertices in $\mathcal{V}$). Therefore,

$$Kd - ||\tilde{c}||_2||u||_2 \leq c_K^T x_K^* = c_K^T \bar{x}_K^* = K\bar{x}_K^*(1) + \tilde{c}^T \bar{x}_K^*(2{:}n) \leq c_K^T x^f \leq Ks + ||\tilde{c}||_2||u||_2,$$

which is absurd for any $K > \frac{2||\tilde{c}||_2||u||_2}{d-s}$. □

The linear program (2) can be written in the form of (10); in fact, $0 \leq X \leq 1$ while the mn additional variables necessary to express the constraint $||M - MX||_1 \leq 2\epsilon$ linearly will be in the interval $[0, 2\epsilon]$. Therefore, Lemma 7 applies to (2).

Proof of Theorem 3. We prove the result with the following construction: Let

$$W = \begin{pmatrix} \frac{\kappa}{2} I_r \\ (1 - \frac{\kappa}{2})e^T \end{pmatrix},$$

which is κ-robustly conical. Let also

$$H = \begin{pmatrix} I_r & \beta I_r + (E_r - I_r)\frac{1-\beta}{r-1} \end{pmatrix},$$

so that $||H'||_\infty = \beta$ (note that β must be larger than $\frac{1}{r}$ since the columns of H' sum to one), $N = 0$, $\tilde{M} = WH + N$, $p = (1, 2, 3, \dots, r-1, -K, -1, -2, \dots, -(r-1), -K^2)^T$ for K sufficiently large, and

$$\epsilon = \frac{\kappa(1-\beta)}{(r-1)(1-\beta)+1} \leq \frac{\kappa}{r-1}.$$

Assume that

$$X = \begin{pmatrix} (1-\delta)I_{r-1} + \frac{\delta-\omega}{r-1}\left(E_{r-1} - I_{r-1}\right) & 0 & (1-\delta)\left(\beta I_{r-1} + \frac{1}{r-1}(E_{r-1} - I_{r-1})\left(\frac{1-\omega}{1-\delta} - \beta\right)\right) & 0 \\ \frac{\delta-\omega}{r-1} e^T & 1 & \frac{1-\delta}{r-1}\left(\frac{1-\omega}{1-\delta} - \beta\right) e^T & 0 \\ \omega I_{r-1} & 0 & \omega I_{r-1} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where

$$\delta = (2-\beta)\omega \quad \text{and} \quad \omega = \frac{\epsilon}{\kappa(1-\beta)}, \qquad \text{implying } X(n,n) = \omega + (r-1)(\delta - \omega) = 1,$$

is a feasible solution of (2) (note that $n = 2r$). By Lemma 7, there exists K sufficiently large such that any optimal solution X^* must satisfy $X^*(n,n) = 1$. Using Lemma 7 again, there exists K sufficiently large such that $X^*(r,r) = 1$. Therefore, for K sufficiently large, the rth and nth column of $\tilde{M}$ will be extracted implying

$$||W - \tilde{W}(:,P)||_1 = \min_{1 \leq j \leq r-1} ||W(:,j) - M(:,n)||_1 = ||W(:,1) - M(:,n)||_1 = \kappa\frac{r-2+\beta}{r-1} > \frac{r-2}{r-1}\kappa \geq \epsilon,$$

and the proof will be complete.

It remains to show that X is feasible: Clearly, $\text{tr}(X) = r$. For the constraints $0 \leq X \leq 1$, we check that

$$0 \leq \omega = \frac{\epsilon}{\kappa(1-\beta)} = \frac{1}{r(1-\beta)+1} \leq \delta = (2-\beta)\omega = \frac{(1-\beta)+1}{r(1-\beta)+1} \leq 1,$$

and

$$0 \leq \frac{1}{r-1}\left(\frac{1-\omega}{1-\delta} - \beta\right) \leq 1 \quad \text{ since } \frac{1-\omega}{1-\delta} = \frac{r-1}{r-2} \geq 1.$$

For $X(i,j) \leq X(i,i)$ for all i,j, we only have to check that

$$1 - \delta \geq \frac{\delta-\omega}{r-1} \iff (r-1)(r-2)(1-\beta) \geq (1-\beta).$$

It remains to verify that $||M(:,j) - MX(:,j)||_1 \leq 2\epsilon$ for all $1 \leq j \leq 2r$:

- $1 \leq j \leq r-1$. We have

$$\begin{aligned} ||M(:,j) - MX(:,j)||_1 &= \left\| M(:,j) - (1-\delta)M(:,j) - \frac{\delta-\omega}{r-1}M(:,j+r) \right\|_1 \\ &= \left\| \delta M(:,j) - \omega M(:,j+r) - \frac{\delta-\omega}{r-1}M(:,\mathcal{J})e \right\|_1 \\ &= \omega \left\| M(:,j) - M(:,j+r) \right\|_1 + (\delta-\omega)\left\| M(:,j) - \frac{1}{r-1}M(:,\mathcal{J})e \right\|_1 \\ &= \omega\kappa(1-\beta) + (\delta-\omega)\kappa \\ &= 2\omega\kappa(1-\beta) = 2\epsilon, \end{aligned}$$

  where $\mathcal{J} = \{1, 2, \dots, r\} \backslash \{j\}$.

- $r+1 \le j \le 2r-1$. We have

$$
\begin{aligned}
||M(:,j) - MX(:,j)||_1 &= \|M(:,j) - \omega M(:,j) - (1-\delta)\beta W(:,j-r) - (1-\omega-\beta(1-\delta))\, w_j\|_1 \\
&= (1-\omega)\left\| M(:,j) - \frac{r-2}{r-1}\beta M(:,j-r) - \left(1-\beta\frac{r-2}{r-1}\right) w_j \right\|_1 \\
&= (1-\omega)\left\| M(:,j) - \left(1-\frac{1}{r-1}\right)\beta W(:,j-r) - \left(1-\beta+\beta\frac{1}{r-1}\right) w_j \right\|_1 \\
&= \frac{\beta(1-\omega)}{r-1}\|W(:,j-r) - w_j\|_1 = \frac{\beta(1-\omega)\kappa}{r-1} \le \frac{(1-\omega)\kappa}{r} \\
&= \frac{(r-1)(1-\beta)\kappa}{r((r-1)(1-\beta)+1)} \le \frac{(1-\beta)\kappa}{(r-1)(1-\beta)+1} = \epsilon,
\end{aligned}
$$

where $w_j = W(:,\mathcal{R})\frac{e}{r-1}$ and $\mathcal{R} = \{1,2,\dots,r\}\backslash\{j-r\}$. In fact, $\frac{1-\delta}{1-\omega} = \frac{r-2}{r-1}$, $\beta \le \frac{1}{r}$, and, by construction, $M(:,j) = \beta W(:,j-r) + (1-\beta)w_j$.

□

Appendix C. Proof of Theorem 6

Proof of Theorem 6. We prove the result with the following construction: Let

$$
W = \begin{pmatrix} \frac{\kappa}{2} I_r \\ (1-\frac{\kappa}{2})e^T \\ 0_{r\times r} \end{pmatrix},
$$

$$
H = \begin{pmatrix} I_{r-1} & 0 & \lambda I_{r-1} & \frac{1}{r-1}e \\ 0 & 1 & (1-\lambda)e^T & 0 \end{pmatrix},
$$

where $\lambda = 2\frac{\epsilon}{\kappa}$,

$$
N = \begin{pmatrix} 0_{(r+1)\times r} & 0_{(r+1)\times 1} & 0_{(r+1)\times(r-1)} & 0_{(r+1)\times 1} \\ \epsilon e^T & 0 & 0_{1\times(r-1)} & \epsilon \\ 0_{(r-1)\times(r-1)} & 0_{(r-1)\times 1} & Z & 0_{(r-1)\times 1} \end{pmatrix},
$$

where $Z = xI_{r-1} + y(E_{r-1} - I_{r-1})$ with $x = \frac{1}{r-1}\epsilon$ and $y = \frac{-x}{r-2}$. The matrix Z has been constructed so that $||Z(:,j)||_1 \le \epsilon$ for all j, $\sum_j Z(i,j) = 0$ for all i, and $\left\|\tilde{M}(:,j) - \frac{1}{r-1}\tilde{M}(:,\mathcal{I})e\right\|_1 = 2\epsilon$ for all $j \in \mathcal{J} = \{r+1, r+2, \dots 2r-1\}$ and $\mathcal{I} = \mathcal{J}\backslash\{i\}$. Let also $\tilde{M} = WH + N$,

$$
\frac{\kappa}{(r-1)^2} < \epsilon \le \frac{\kappa}{2(r-1)} \quad \text{so that } \lambda \le \frac{1}{r-1},
$$

and

$$
p = (1, 2, \dots, r-1, K^3, K^2, K^2+1, \dots, K^2+r-1, -K)^T,
$$

for K sufficiently large. Assume

$$
X = \begin{pmatrix} (1-\frac{2\epsilon}{\kappa})I_{r-1} & 0 & \lambda\frac{r-2}{r-1}I_{r-1} & \left(1-\frac{2\epsilon(r-1)}{\kappa}\right)e \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1}{r-1}e & \frac{1}{r-1}E_{r-1} & 0 \\ \frac{2\epsilon}{\kappa}e^T & 0 & 0 & (r-1)\frac{2\epsilon}{\kappa} \end{pmatrix},
$$

is feasible for (2). Letting X^* be any optimal solution, by Lemma 7, there exists K sufficiently large such that $X^*(r,r) = 0$. By Lemma 8 (see below), this implies that $X^*(j,j) \ge \frac{1}{r-1}$ for $j \in \mathcal{J}$.

Using Lemma 7 again, we have that for K sufficiently large $X^*(j,j) = \frac{1}{r-1}$ for all for $j \in \mathcal{J}$, and $X^*(n,n) \geq (r-1)\frac{2\epsilon}{\kappa}$. Therefore, since

$$\frac{2\epsilon(r-1)}{\kappa} > \frac{1}{r-1} \iff \epsilon > \frac{\kappa}{2(r-1)^2}, \quad \text{and} \quad 1 - \frac{2\epsilon}{\kappa} > \frac{1}{r-1} \iff \epsilon < \left(\frac{r-2}{r-1}\right)\frac{\kappa}{2} \leq \frac{\kappa}{4},$$

the first $r-1$ columns and the last column of $\tilde{M}$ will be extracted so that

$$||W - \tilde{W}||_1 = ||W(:,r) - \tilde{M}(:,n)||_1 = \kappa + \epsilon,$$

and the proof will be complete.

It remains to show that X is feasible. We clearly have $\text{tr}(X) = r$, $0 \leq X \leq 1$, and $X(i,j) \leq X(i,i)$ for all i,j because $\epsilon \leq \frac{\kappa}{2(r-1)}$ while, for $||\tilde{M}(:,j) - \tilde{M}X(:,j)||_1 \leq 2\epsilon$ for all j, we have

- $1 \leq j \leq r-1$.

$$||\tilde{M}(:,j) - \tilde{M}X(:,j)||_1 = \frac{2\epsilon}{\kappa}||\tilde{M}(:,j) - \tilde{M}(:,n)||_1 = 2\frac{r-2}{r-1}\epsilon \leq 2\epsilon.$$

- $j = r$. This follows from Lemma 8.
- $r+1 \leq j \leq 2r-1$. This follows from the construction of matrix Z.
- $j = 2r$. $\tilde{M}(:,j) = \tilde{M}X(:,j)$ since $\tilde{M}(:,j) = \frac{1}{r-1}W(:,1{:}r-1)e$.

□

Lemma 8. *Let W, H, N and $\tilde{M} = WH + N$ be the matrices constructed in Theorem 6. Let also $\mathcal{R} = \{1,2,\ldots,n\}\backslash\{r\}$. Then*

$$\min_{x \geq 0} ||\tilde{M}(:,r) - \tilde{M}(:,\mathcal{R})x||_1 = 2\epsilon, \tag{11}$$

and the unique *optimal solution of* (11) *is given by*

$$x^\dagger = \begin{pmatrix} 0_{(r-1)\times 1} \\ \frac{1}{r-1}e \\ 0_{1\times 1} \end{pmatrix} \in \mathbb{R}^{2r-1}.$$

Proof. Let $x^* = (y,z,w)$ be an optimal solution of (11) where $y, z \in \mathbb{R}^{r-1}_+$ and $w \in \mathbb{R}_+$. We have to show that $x^* = x^\dagger$. From x^*, let us construct another optimal solution $x' = (y', z', 0)$ such that all the entries of y' and z' are equal to each other. Because $\tilde{M}(:,n) = \frac{1}{r-1}\tilde{M}(:,1{:}r-1)e$, we take $w = 0$, replace $z \leftarrow z + \frac{w}{r-1}$ and obtain an equivalent solution. Let us denote $\bar{\mathcal{R}} = \mathcal{R}\backslash\{n\}$ and

$$g(y,z) = \left\|\tilde{M}(:,r) - \tilde{M}(:,\bar{\mathcal{R}})\begin{pmatrix} y \\ z \end{pmatrix}\right\|_1.$$

By symmetry, one can check that $g(y,z) = g(y(P), z(P))$ for any permutation P of $\{1,2,\ldots,r-1\}$ (this simply amounts to permuting the first and last $r-1$ columns of $M(:,\bar{\mathcal{R}})$). By convexity, $(y', z') = \frac{1}{|\Pi|}\sum_{P \in \Pi}(y(P), z(P))$, where Π is the set of all possible permutations of $\{1,2,\ldots,r-1\}$, is also an optimal solution of (11) hence all entries of y' and z' are equal to each other, and $||y'||_1 = ||y||_1$ and $||z'||_1 = ||z||_1$.

Therefore, denoting $y'(i) = \frac{a}{r-1}$ and $z'(i) = \frac{b}{r-1}$ for all $1 \leq i \leq r-1$, the optimization problem (11) can be reduced to

$$\min_{a,b \geq 0} \left\| \begin{pmatrix} 0_{(r-1)\times 1} \\ \frac{\kappa}{2} \\ 1 - \frac{\kappa}{2} \\ 0 \\ 0_{(r-1)\times 1} \end{pmatrix} - a \begin{pmatrix} \frac{\kappa}{2(r-1)}e \\ 0 \\ 1 - \frac{\kappa}{2} \\ \epsilon \\ 0_{(r-1)\times 1} \end{pmatrix} - b \begin{pmatrix} \frac{\lambda\kappa}{2(r-1)}e \\ (1-\lambda)\frac{\kappa}{2} \\ 1 - \frac{\kappa}{2} \\ 0 \\ 0_{(r-1)\times 1} \end{pmatrix} \right\|_1 \tag{12}$$

$$\equiv \min_{a,b\geq 0} \; h(a,b) = \frac{\kappa}{2}\left|a+\lambda b\right| + \frac{\kappa}{2}\left|1-(1-\lambda)b\right| + \left(1-\frac{\kappa}{2}\right)\left|1-a-b\right| + \epsilon\left|a\right|.$$

Let us show that $(a^*,b^*) = (0,1)$ is the unique optimal solution, for which $h(0,1) = \kappa\lambda = 2\epsilon$. For $a+b > 1$, the subdifferential of h in a is $1-\epsilon > 0$, while, for $a+b < 1$, the subdifferential of h in b is $\kappa\lambda - 1 < 0$ hence $a^* + b^* = 1$ at optimality. Substituting $a = 1-b$ above, we obtain

$$b^* = \operatorname{argmin}_{0\leq b\leq 1} \; 2|1-(1-\lambda)b| = 1,$$

which is unique as the slope at $b = 1$ is positive.

Finally, we have $b^* = 1$, $a^* = 0$ is the unique solution of (12) implying that $y' = y = 0$ and that the minimal objective function value of (11) is 2ϵ. Moreover, this implies $||z'||_1 = ||z||_1 = 1$. It remains to show that the entries of z are equal to each other, that is, show that the unique solution to the following system

$$\left\| \begin{pmatrix} 0_{(r-1)\times 1} \\ \frac{\kappa}{2} \\ 0_{(r-1)\times 1} \end{pmatrix} - \begin{pmatrix} \frac{\lambda\kappa}{2} I_{r-1} \\ (1-\lambda)\frac{\kappa}{2} \\ Z \end{pmatrix} z \right\|_1 = 2\epsilon,$$

is $z^* = \frac{1}{r-1}e$, which is clearly the case as the only z such that $Zz = 0$ and $||z||_1 = 1$ is z^*. This completes the proof. □

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