Exact Nonnegative Matrix Factorization via Conic Optimization

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Abstract

In this paper, we present two new approaches for computing exact nonnegative matrix factorizations (NMFs). Exact NMF can be defined as follows: given an input nonnegative matrix \( V \in \mathbb{R}^{F \times N}_+ \) and a factorization rank \( K \), compute, if possible, two nonnegative matrices, \( W \in \mathbb{R}^{F \times K}_+ \) and \( H \in \mathbb{R}^{K \times N}_+ \), such that \( V = WH \). The two proposed approaches to tackle exact NMF, which is NP-hard in general, rely on the same two steps. First, we reformulate exact NMF as minimizing a concave function over a product of convex cones; one approach is based on the exponential cone, and the other on the second-order cone. Second, we solve these reformulations iteratively: at each step, we minimize exactly, over the feasible set, a majorization of the objective functions obtained via linearization at the current iterate. Hence these subproblems are convex conic programs and can be solved efficiently using dedicated algorithms. We show that our approaches, which we call successive conic convex approximations, are able to compute exact NMFs, and compete favorably with the state of the art when applied to several classes of nonnegative matrices; namely, randomly generated, infinite rigid and slack matrices.

Keywords. exact nonnegative matrix factorization, exponential cone, second-order cone, concave minimization, conic optimization.

1 Introduction

Nonnegative matrix factorization (NMF) is the problem of approximating a given nonnegative matrix, \( V \in \mathbb{R}^{F \times N}_+ \), as the product of two smaller nonnegative matrices, \( W \in \mathbb{R}^{F \times K}_+ \) and \( H \in \mathbb{R}^{K \times N}_+ \), where \( K \) is a given parameter known as the factorization rank. One aims at finding the best approximation, that is, the one that minimizes the discrepancy between \( V \) and the product \( WH \), often measured by the Frobenius norm of their difference, \( \| V - WH \|_F \). Despite the fact that NMF is NP-hard in general [10] (see also [14]), it has been used successfully in many domains such as probability, geoscience, medical imaging, computational geometry, combinatorial optimization, analytical chemistry, and machine learning; see [6, 7] and the references therein. Many local optimization schemes have been developed to compute NMFs. They aim to identify local minima or stationary points of optimization problems that minimize the discrepancy between \( V \) and the approximation \( WH \). Most of

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these iterative algorithms rely on a two-step block coordinate descent (BCD) scheme that consists in (approximatively) optimizing alternatively over $W$ with $H$ fixed, and vice-versa. Comparatively, less attention has been given in the literature to the development of algorithms aimed at finding global minima of the optimization problems associated to NMF models. In this paper, we are interested in computing high quality local minima for the NMF optimization problems without relying on the BCD framework. We will perform the optimization over $W$ and $H$ jointly. Moreover, our focus is on finding exact NMFs, that is, computing nonnegative factors $W$ and $H$ such that $V = WH$, although our approaches can be used to find approximate NMFs.

The minimum factorization rank $K$ for which an exact NMF exists is called the nonnegative rank of $V$ and is denoted $\text{rank}_+(V)$, we have

$$\text{rank}_+(V) = \min \left\{ K \in \mathbb{N} \mid V = WH, W \in \mathbb{R}_+^{F \times K} \text{ and } H \in \mathbb{R}_+^{K \times N} \right\}.$$

The computation of the nonnegative rank is NP-hard [16], and is a research topic on its own; see [7, Chapter 3], [5] and the references therein for recent progress on this question.

### 1.1 Computational complexity

Solving exact NMF can be used to compute the nonnegative rank, by finding the smallest $K$ such that an exact NMF exists. Cohen and Rothblum [4] give a super-exponential time algorithm for this problem. Vavasis [16] proved that checking whether $\text{rank}(V) = \text{rank}_+(V)$, where $\text{rank}(V) = K$ is part of the input, is NP-hard. Therefore, unless $P=NP$, no algorithm can solve exact NMF using a number of arithmetic operations bounded by a polynomial in $K$ and in the size of $V$; see also [14] that gives a different proof using algebraic arguments.

More recently, Arora et al. [1] showed that no algorithm to solve this problem can run in time $(FN)^{o(K)}$ unless 3-SAT can be solved in time $2^{o(n)}$ on instances with $n$ variables. However, in practice, $K$ is small and it makes senses to wonder what is the complexity if $K$ is assumed to be a fixed constant. In that case, they showed that exact NMF can be solved in polynomial time in $F$ and $N$, namely in time $O((FN)^{cK^2})$ for some constant $c$, which Moitra [12] later improved to $O((FN)^{cK^2})$.

The argument is based on the quantifier elimination theory, using the seminal result by Basu, Pollack and Roy [2]. Unfortunately, this approach cannot be used in practice even for small size matrices because of its high computational cost: although the term $O((FN)^{cK^2})$ is a polynomial in $F$ and $N$ for $K$ fixed, it grows extremely fast (and the hidden constants are usually very large). Therefore developing an effective computational technique for exact NMF of small matrices is an important direction of research. Some heuristics have been recently developed that allow solving exact NMF for matrices up to a few dozen rows and columns [15].

### 1.2 Contribution and outline of the paper

In this paper, we introduce two approaches for computing an exact NMF using conic optimization. They rely on the same two steps. First, in Section 2, we reformulate exact NMF as minimizing a concave function over a product of convex cones; one approach is based on the exponential cone, and the other on the second-order cone. Then, in Section 3, we solve these reformulations iteratively: at each step, we minimize exactly, over the feasible set, a majorization of the objective functions obtained

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3-SAT, or 3-satisfiability, is an instrumental problem in computational complexity to prove NP-completeness results. 3-SAT is the problem of deciding whether a set of disjunctions containing 3 Boolean variables or their negation can be satisfied.
via linearization at the current iterate. Hence these subproblems are convex conic programs and can be solved efficiently using dedicated algorithms. Finally, in Section 4 we show that our approaches are able to compute exact NMFs and compete favorably with the state of the art when applied to several classes of nonnegative matrices; namely, randomly generated, infinitesimally rigid and slack matrices.

2 Reformulations of exact NMF based on conic optimization

In this section we propose two new formulations for the exact NMF model, $V = WH$ with $(W,H) \geq 0$, where the feasible set is represented using the exponential cone (Section 2.1) and the second-order cone (Section 2.2).

2.1 NMF formulation via exponential cones

Our first proposed formulation is the following:

$$\max_{W \in \mathbb{R}^{F \times K}, H \in \mathbb{R}^{K \times N}} \sum_{f=1}^{F} \sum_{n=1}^{N} \sum_{k=1}^{K} W_{fk} H_{kn}$$

subject to

$$\sum_{k=1}^{K} W_{fk} H_{kn} \leq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},$$

$$W_{fk} \geq 0, H_{kn} \geq 0 \text{ for } f \in \mathcal{F}, k \in \mathcal{K}, n \in \mathcal{N}.$$  (1)

where $\mathcal{F} = \{1, \ldots, F\}$, $\mathcal{N} = \{1, \ldots, N\}$ and $\mathcal{K} = \{1, \ldots, K\}$. Any feasible solution $(W,H)$ of (1) provides an under-approximation of $V$, because of the elementwise constraint $WH \leq V$. The objective function of (1) maximizes the sum of the entries of $WH$. Therefore, if $V$ admits an exact NMF of size $K$, that is, $\text{rank}_+(V) \leq K$, any optimal solution $(W^*,H^*)$ of (1) must satisfy $W^* H^* = V$, and hence will provide an exact NMF of $V$. Note that this problem is nonconvex because of the bilinear terms appearing in the objective and the constraint $WH \leq V$.

Let us now reformulate (1) using exponential cones. In order to deal with nonnegativity constraints on the entries of $W$ and $H$, we use the following change of variables: $W_{fk} = G(U_{fk}) = e^{U_{fk}}$ and $H_{kn} = G(T_{kn}) = e^{T_{kn}}$, where $U \in \mathbb{R}^{F \times K}$ and $T \in \mathbb{R}^{K \times N}$, with $f = 1, \ldots, F$, $n = 1, \ldots, N$ and $k = 1, \ldots, K$ and $G(t) = e^t$. By applying a logarithm on top of this change of variables to the objective function, and on both sides of the inequality constraints $WH \leq V$, (1) can be nearly equivalently rewritten as follows, the difference being that zero elements in $W$ and $H$ are now excluded:

$$\max_{U \in \mathbb{R}^{F \times K}, T \in \mathbb{R}^{K \times N}} \log \left( \sum_{f,n,k} e^{U_{fk} + T_{kn}} \right)$$

subject to

$$\log \left( \sum_{k=1}^{K} e^{U_{fk} + T_{kn}} \right) \leq \log (V_{fn}) \text{ for } f \in \mathcal{F}, n \in \mathcal{N};$$  (2)

which corresponds to the maximization of a convex function (logarithm of the sums of exponentials) over a convex set, each constraint is convex for the same reason. We rewrite the convex feasible set of
with explicit conic constraints as follows:
\[
\sum_{k=1}^{K} t_{fkn} \leq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
\]
\[
(t_{fkn}, 1, U_{fk} + T_{kn}) \in K_{exp} \text{ for } f \in \mathcal{F}, k \in \mathcal{K}, n \in \mathcal{N},
\]
where \( K_{exp} \subset \mathbb{R}^3 \) denotes the (primal) exponential cone defined as:
\[
K_{exp} = \left\{ (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_1 \geq x_2 e^{x_3}, x_2 > 0 \right\} \cup \{ (x_1, 0, x_3) \mid x_1 \geq 0, x_3 \leq 0 \}. \tag{4}
\]
Note that the exponential cone is closed and includes the subset \( \{ (x_1, 0, x_3) \mid x_1 \geq 0, x_3 \leq 0 \} \), therefore the scenarios for which the entries \( V_{fn} \) are equal to zero can be handled by exponential conic constraints, which was not possible with formulation (2) since the log function is not defined at zero. Hence the optimization problem (1) can be written equivalently as
\[
\max_{U \in \mathbb{R}^{F \times K}, T \in \mathbb{R}^{K \times N}, A \in \mathbb{R}^{F \times K \times N}} \log \left( \sum_{f,n,k} e^{U_{fk} + T_{kn}} \right)
\]
subject to
\[
\sum_{k=1}^{K} t_{fkn} \leq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
\]
\[
(t_{fkn}, 1, U_{fk} + T_{kn}) \in K_{exp} \text{ for } f \in \mathcal{F}, k \in \mathcal{K}, n \in \mathcal{N}.
\]
This leads to \( F \times N \) inequality constraints and the introduction of \( F \times K \times N \) exponential cones. In Section 3, we propose an algorithm to tackle (5) using successive linearizations of the objective function.

### 2.2 NMF formulation via rotated second-order cones

Our second proposed formulation is the following:
\[
\min_{W \in \mathbb{R}^{F \times K}, H \in \mathbb{R}^{K \times N}} \sum_{f=1}^{F} \sum_{n=1}^{N} \left( \sum_{k=1}^{K} W_{fk} H_{kn} \right)
\]
subject to
\[
\sum_{k=1}^{K} W_{fk} H_{kn} \geq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
\]
\[
W_{fk}, H_{kn} \geq 0 \text{ for } f \in \mathcal{F}, k \in \mathcal{K}, n \in \mathcal{N}.
\]
Any feasible solution \((W, H)\) of (6) provides an over-approximation of \( V \), because of the constraint \( WH \geq V \). The objective function of (11) minimizes the sum of the entries of \( WH \). Therefore, if \( \text{rank}_+(V) \leq K \), any optimal solution \((W^*, H^*)\) of (11) must satisfy \( W^* H^* = V \), and hence will provide an exact NMF of \( V \). Again the problem is nonconvex due to the bilinear terms.

Let us use the following change of variables: we pose \( W_{fk} = G(U_{fk}) = \sqrt{U_{fk}} \) and \( H_{kn} = G(T_{kn}) = \sqrt{T_{kn}} \) where \( U \in \mathbb{R}_+^{F \times K} \) and \( T \in \mathbb{R}_+^{K \times N} \), with \( f = 1, \ldots, F, n = 1, \ldots, N \) and \( k = 1, \ldots, K \), this time
with $G(t) = \sqrt{t}$. Thus the optimization problem (6) can be equivalently rewritten as:

$$
\min_{U \in \mathbb{R}^{F \times K}, T \in \mathbb{R}^{K \times N}} \sum_{f=1}^{F} \sum_{n=1}^{N} \left( \sum_{k=1}^{K} \sqrt{U_{fk}} \sqrt{T_{kn}} \right)
$$

subject to

$$
\sum_{k=1}^{K} \sqrt{U_{fk}} \sqrt{T_{kn}} \geq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
$$

which minimizes a concave function over a convex set. Indeed, the function $\sqrt{xy}$ is concave. This set can be written with conic constraints as follows:

$$
\sum_{k=1}^{K} t_{fkn} \geq V_{fn}, \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
$$

where $Q^3_r$ denotes the 3-dimensional rotated second-order cone defined as:

$$
Q^3_r = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid 2x_1 x_2 \geq x_3, x_1 \geq 0, x_2 \geq 0\}.
$$

Thus, the optimization problem (7) becomes

$$
\min_{U \in \mathbb{R}^{F \times K}, T \in \mathbb{R}^{K \times N}, t \in \mathbb{R}^{F \times K \times N}} \sum_{f=1}^{F} \sum_{n=1}^{N} \left( \sum_{k=1}^{K} \sqrt{U_{fk}} \sqrt{T_{kn}} \right)
$$

subject to

$$
\sum_{k=1}^{K} t_{fkn} \geq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
$$

where $Q^3_r$ denotes the 3-dimensional rotated second-order cone defined as:

$$
Q^3_r = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid 2x_1 x_2 \geq x_3, x_1 \geq 0, x_2 \geq 0\}.
$$

Thus, the optimization problem becomes

$$
\min_{U \in \mathbb{R}^{F \times K}, T \in \mathbb{R}^{K \times N}, t \in \mathbb{R}^{F \times K \times N}} \sum_{f=1}^{F} \sum_{n=1}^{N} \left( \sum_{k=1}^{K} \sqrt{U_{fk}} \sqrt{T_{kn}} \right)
$$

subject to

$$
\sum_{k=1}^{K} t_{fkn} \geq V_{fn} \text{ for } f \in \mathcal{F}, n \in \mathcal{N},
$$

which leads to $F \times N$ inequality constraints and the introduction of $F \times K \times N$ rotated quadratic cones.

**3 A successive linearization algorithm**

In this section, we present an iterative algorithm to tackle problems (5) and (9). Both problems can be written as the minimization of a concave function $\Phi$ over a convex set denoted by $Q$. Note that $Q$ designates either the feasible set of (5) or the feasible set of (9).

This minimization is performed by solving a sequence of simpler problems in which the objective function is replaced by its linearization constructed at the current solution $(U, T)$. Let us denote $Z^i = (U^i, T^i)$ the $i$th iterate of our algorithm. At each iteration $i$, we update $Z$ as follows:

$$
Z^i \in \arg\min_{Z \in Q} \Phi(Z^{i-1}) + \langle \nabla \Phi(Z^{i-1}), Z - Z^{i-1} \rangle
$$

$$
\in \arg\min_{Z \in Q} \langle \nabla \Phi(Z^{i-1}), Z \rangle,
$$

(10)
where $\Phi$ is the objective function of (5) or (9). Since the objective of (10) is linear in $Z$, the subproblems become convex. Moreover they are particular structured conic optimization problems. In this paper, we use the MOSEK software [13] to solve each successive problem (10) with an interior-point method (IPM). Algorithm 1 summarizes our proposed method to tackle (5) and (9).

To initialize $U$ and $T$, we chose to randomly initialize $W$ and $H$ (using the uniform distribution in the interval $[0, 1]$ for each entry of $W$ and $H$) and apply the two changes of variables, $G(\cdot)$, to compute the initializations for $U$ and $T$.

A final refinement step further improves the output of the main algorithm using the state-of-the-art accelerated HALS algorithm, an exact BCD method for NMF, from [8]. In this paper, we use a tolerance for the relative error equal to $10^{-6}$, that is, we assume that an exact NMF $(W, H)$ is found for an input matrix $V$ as soon as $\frac{\|V - WH\|_F}{\|V\|_F} \leq 10^{-6}$. This is the same refinement strategy as used in [15].

**Algorithm 1** Successive Conic Convex Approximation for Exact NMF

**Input:** Input matrix $V \in \mathbb{R}^{F \times N}_+$, the factorization rank $K$, number of iterations $\text{maxiter}$.

**Output:** $(W, H) \geq 0$ is such that $V = WH$ with $\frac{\|V - WH\|_F}{\|V\|_F} \leq 10^{-6}$.

1: % Block 1: Initialization
2: $(W^0, H^0) \leftarrow$ positive random initialization($F, K, N$).
3: $(U^0, T^0) \leftarrow G^{-1}(W^0, H^0)$ where $G$ is the change of variables
4: $Z^0 \leftarrow (U^0, T^0)$
5: % Block 2: iterative update of $Z$
6: for $i = 1, 2, \ldots, \text{maxiter}$ do
7: \hspace{1em} $Z^i \leftarrow \arg\min_{Z \in Q} \langle \nabla \Phi(Z^{i-1}), Z \rangle_F$ with IPM available in MOSEK [13]
8: end for
9: $(W, H) \leftarrow G(Z^i)$
10: % Block 3: Final Refinement
11: $(W, H) \leftarrow \text{Algo A-HALS}(V, W, H)$ from [8]

**Discussion on convergence** Since $\Phi(Z)$ is concave, its linearization provides an upper approximation, that is, $\Phi(Z^{i-1}) + \langle \nabla \Phi(Z^{i-1}), Z - Z^{i-1} \rangle \geq \Phi(Z)$ for all $Z \in Q$, which is exactly minimized over the feasible set $Q$ at each iteration. This implies that $\Phi(Z)$ is nonincreasing under the updates of Algorithm 1. Since $\Phi(Z)$ is bounded below on $Q$, by construction, the sequence of objective function values $\{\Phi(Z^i)\}$ converges. It is however not guaranteed to tend to a global minimum. Further works will focus on the convergence analysis of the sequence of iterates $\{Z^i\}$ generated by Algorithm 1 in particular convergence to a stationary point.

### 4 Numerical experiments

In this section, Algorithm 1 is tested for the computation of exact NMF for particular classes of matrices usually considered in the literature: (1) 10-by-10 matrices randomly generated with nonnegative rank 5 (each matrix is generated by multiplying two random rank-5 nonnegative matrices), (2) four 6-by-6 infinitesimally rigid factorizations with nonnegative rank 5 [10], denoted $V_{\text{inf}}^i$ for $i = 1, 2, 3, 4$, and (3) four 5-by-5 slack matrices corresponding to nested hexagons, denoted $V_{\text{a=\pi}}^i$, with nonnegative
ranks 3, 4, 5, 5 depending on a parameter $x = 2, 3, 4, +\infty$, respectively. These matrices are described in more details in the Appendix.

For each of the matrices, we run Algorithm 1 for 750 iterations for nested hexagons and random matrices, and 3000 iterations for infinitesimally rigid matrices, and the state-of-the-art algorithm from [15] with Multi-Start 1 heuristic "ms1" and the Rank-by-rank heuristic "rbr". For each method, we run 100 initializations with SPARSE10, as recommended in [15], with target precision $10^{-6}$. Note that a different random matrix is generated each time for the experiments on random matrices, following the procedure described in the Appendix.

Table 1 reports the number of successes over 100 attempts for computing the exact NMF of the input matrices defined as obtaining a solution where $\frac{\|V-WH\|_F}{\|V\|_F}$ is below the target precision, namely $10^{-6}$.

Table 1: Comparison of the two variants of Algorithm 1 for (5) and (9) with the algorithm from [15] with the "ms1" and "rbr" heuristics. Each run is performed with 100 initializations to compute the factorizations of matrices described in the Appendix. In bold, we indicate the algorithm that found the most exact NMFs.

| Matrices       | Algorithm 1 for (5) /100 | Algorithm 1 for (9) /100 | Algorithm from [15] with "ms1" /100 | Algorithm from [15] with "rbr" /100 |
|---------------|--------------------------|--------------------------|------------------------------------|-----------------------------------|
| Random matrices |                          |                          |                                    |                                   |
| Inf. Rig. Fac. |                          |                          |                                    |                                   |
| $V_{inf1}$     | 5                        | 7                        | 4                                  | 0                                 |
| $V_{inf2}$     | 45                       | 42                       | 34                                 | 97                                |
| $V_{inf3}$     | 14                       | 29                       | 14                                 | 90                                |
| $V_{inf4}$     | 15                       | 23                       | 15                                 | 0                                 |
| Nested hexagons |                          |                          |                                    |                                   |
| $V_{a=2}$      | 100                      | 100                      | 100                                | 100                               |
| $V_{a=3}$      | 100                      | 100                      | 100                                | 100                               |
| $V_{a=4}$      | 36                       | 64                       | 36                                 | 100                               |
| $V_{a\to+\infty}$ | 17                      | 38                       | 20                                 | 100                               |

We observe the following:

- All algorithms find exact NMFs in each run for random matrices. It is well-known that factorizing randomly generated matrices is typically easier [15]. This shows that Algorithm 1 with both formulations (5) and (9) is also able to compute exact NMFs in this scenario, which is reassuring.

- Looking at the nonrandom matrices, Algorithm 1 with both formulations (5) and (9), and "ms1" from [15] are the only algorithms able to compute an exact NMF for at least some of the 100 initializations. Moreover, among these three algorithms, Algorithm 1 with (9) found most frequently an exact NMF, except for $V_{inf2}$ where Algorithm 1 with (5) found 45 exact NMFs while with (9) only found 42.

- For some matrices (namely, $V_{a=4}$ and $V_{a\to+\infty}$), "rbr" from [15] is able to compute exact NMF for all initializations, which is not the case of the other algorithms. However, "rbr" is not able to compute exact NMFs for $V_{inf1}$ and $V_{inf2}$.
In summary, Algorithm 1 competes favorably with the algorithms proposed in [15], and appears to be more robust in the sense that it computes exact NMFs in all the tested cases.

Computational time In terms of computational time, Algorithm 1 is slower than the algorithm from [15], and it does not scale as well. The main reason is that it relies on interior-point methods, while [15] relies on first-order methods (more precisely, exact BCD). For example, for the infinitesimally rigid matrices, Algorithm 1 takes on average 30 seconds (resp. 72 seconds) to compute a solution using (5) (resp. using (9)), while [15] takes between 2 and 16 seconds. The difference would be more significant for larger matrices. Hence a possible direction of research would be to use faster methods to tackle the conic optimization problems.

5 Conclusion

In this paper, we introduced two formulations for computing exact NMFs, namely (1) and (6) that are under- and upper-approximation formulations for NMF, respectively. For each formulation, we used a particular change of variables that enabled the use of two convex cones, namely the exponential and second-order cones, to reformulate these problems as the minimization of a concave function over a convex feasible set. In order to solve the two optimization problems, we proposed Algorithm 1 that relies on the resolution of successive linear approximations of the objective functions and the use of interior-point methods. We showed that Algorithm 1 is able to compute exact NMFs for several classes of nonnegative matrices (namely, randomly generated matrices, infinitesimally rigid matrices, and slack matrices of nested hexagons) and as such demonstrate its competitiveness compared to recent methods from the literature. However, we have tested Algorithm 1 on a limited number of nonnegative matrices. In the future we plan to test it on a larger library of nonnegative matrices, in order to better understand the behavior of Algorithm 1 along with the two formulations (5) and (9).

Further works also include:

- The design of more advanced strategies for the initialization of $(U, T)$.
- The elaboration of alternative formulations for (5) and (9) to deal with the non-uniqueness of the NMF models. In particular, we plan to develop new formulations that discard solutions of the form $V = WH = (WE)(E^{-1}H)$ for a given solution $(W, H)$ and for invertible matrices $E$ such that $WE \geq 0$ and $E^{-1}H \geq 0$. For example, one could remove the permutation and scaling ambiguity for the columns of $W$ and rows of $H$, to remove some degrees of freedom in the formulations. We refer the interested reader to [6] and [7, Chapter 4], and the references therein, for more information on the non-uniqueness of NMF.
- The use of our framework for other closely related problems; in particular the computation of symmetric NMFs which requires $H = W^\top$; this problem is closely related to completely positive matrices [3]. Symmetric NMF can be used for data analysis and in particular for various clustering tasks [11].
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Appendix

In this appendix, we describe the matrices considered for the numerical experiments in Section 4:

- **Randomly Generated Matrices:** It is standard in the NMF literature to use randomly generated matrices to compare algorithms (see, e.g., [9]). In this paper, we used the standard approach: $V = WH \in \mathbb{R}_+^{F \times N}$ where each entry of $W \in \mathbb{R}_+^{F \times K}$ and $H \in \mathbb{R}_+^{K \times N}$ is generated using the uniform distribution in the interval $[0, 1]$, and $K \leq \min(F, N)$. With this approach, $\text{rank}(V) = \text{rank}_+(V) = K$ with probability one. In the numerical experiments reported in Section 4, we used $F = N = 10$ and $K = 5$.

- **Infinitesimally rigid factorizations:** in this paper, we consider four infinitesimally rigid factorizations for $5 \times 5$ matrices with positive entries and with nonnegative rank equal to four from [10]:

$$V_{\text{inf1}} = \begin{pmatrix}
573705 & 806520 & 167622 & 246500 & 531659 \\
397096 & 39600 & 299176 & 827468 & 851798 \\
131646 & 403260 & 30269 & 226915 & 264510 \\
9114 & 85160 & 311182 & 827468 & 851798 \\
147857 & 3200 & 351037 & 599025 & 697755
\end{pmatrix},$$

$$V_{\text{inf2}} = \begin{pmatrix}
30893 & 319912 & 149770 & 873 & 111428 \\
383490 & 87990 & 5580 & 628440 & 587250 \\
560076 & 1030324 & 331070 & 288045 & 350647 \\
203830 & 305184 & 277512 & 264376 & 205933 \\
90911 & 142936 & 500784 & 618842 & 609633
\end{pmatrix},$$

$$V_{\text{inf3}} = \begin{pmatrix}
948201 & 723609 & 958755 & 591858 & 397953 \\
222448 & 218040 & 30429 & 348793 & 15825 \\
560076 & 1030324 & 331070 & 288045 & 350647 \\
203830 & 305184 & 277512 & 264376 & 205933 \\
90911 & 142936 & 500784 & 618842 & 609633
\end{pmatrix},$$

$$V_{\text{inf4}} = \begin{pmatrix}
1 & x & 2x - 1 & 2x - 1 & x & 1 \\
1 & 1 & x & 2x - 1 & 2x - 1 & x \\
x & 1 & 1 & x & 2x - 1 & 2x - 1 \\
2x - 1 & x & 1 & 1 & x & 2x - 1 \\
x & 2x - 1 & 2x - 1 & x & 1 & 1 \\
x & 2x - 1 & 2x - 1 & x & 1 & 1
\end{pmatrix}.$$

These matrices have been shown to be challenging to factorize; see [10] for more details.

- **Nested hexagons problem:** computing an exact NMF is equivalent to tackle a well-known problem in computational geometry which is referred to as nested polytope problem. Here we consider a family of input matrices whose exact NMF corresponds to finding a polytope nested between two hexagons; see [7, Chapter 2] and the references therein. Given $x > 1$, $V_{a=x}$ is defined as

$$\frac{1}{x} \begin{pmatrix}
1 & x & 2x - 1 & 2x - 1 & x & 1 \\
1 & 1 & x & 2x - 1 & 2x - 1 & x \\
x & 1 & 1 & x & 2x - 1 & 2x - 1 \\
2x - 1 & x & 1 & 1 & x & 2x - 1 \\
x & 2x - 1 & 2x - 1 & x & 1 & 1 \\
x & 2x - 1 & 2x - 1 & x & 1 & 1
\end{pmatrix}$$

which satisfies $\text{rank}(V_{a=x}) = 3$ for any $x > 1$. The nonnegative rank of $V_{a=x}$ for $x = 2, 3, 4, +\infty$ is $3, 4, 5, 5$, respectively.