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Nonnegative Matrix Factorization Requires Irrationality*

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Abstract. Nonnegative matrix factorization (NMF) is the problem of decomposing a given nonnegative $n \times m$ matrix M into a product of a nonnegative $n \times d$ matrix W and a nonnegative $d \times m$ matrix H. A longstanding open question, posed by Cohen and Rothblum in 1993, is whether a rational matrix M always has an NMF of minimal inner dimension d whose factors W and H are also rational. We answer this question negatively, by exhibiting a matrix for which W and H require irrational entries.

Key words. nonnegative matrix factorization, nonnegative rank

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1. Introduction.

Nonnegative matrix factorization (NMF) is the task of factoring a matrix of nonnegative real numbers M (henceforth a *nonnegative* matrix) as a product $M = W \cdot H$ such that the matrices W and H are also nonnegative. As well as being a natural problem in its own right (see Thomas [26] and Cohen and Rothblum [9]), NMF has found many applications in various domains, including machine learning, combinatorics, and communication complexity; see, e.g., [3, 13, 18, 19, 28, 29] and the references therein.

For an NMF $M = W \cdot H$, the number of columns in W is called the *inner dimension*. The smallest inner dimension of any NMF of M is called the *nonnegative rank (over the reals)* of M; an early reference is the paper by Gregory and Pullman [15]. Similarly, the *nonnegative rank of M over the rationals* is defined as the smallest inner dimension of an NMF $M = W \cdot H$ with matrices W, H that have only *rational* entries. Cohen and Rothblum [9] posed the following problem in 1993:

> "PROBLEM. *Show that the nonnegative ranks of a rational matrix over the reals and over the rationals coincide, or provide an example where the two ranks are different.*"

In this paper, we solve the above problem by providing an example of a rational matrix M that has different nonnegative ranks over $\mathbb{R}$ and over $\mathbb{Q}$.

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Discussion. In the last few years, there has been progress towards resolving the Cohen–Rothblum problem. It was already known to Cohen and Rothblum [9] that the nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ coincide for matrices of rank at most 2. (Note that the usual ranks over $\mathbb{R}$ and $\mathbb{Q}$ coincide for all rational matrices.) In 2015, Kubjas, Robeva, and Sturmfels [16, Corollary 4.6] extended this result to matrices of nonnegative rank (over $\mathbb{R}$) at most 3. On the other hand, Shitov [22] proved that the nonnegative rank of a matrix can indeed depend on the underlying field: he exhibited a nonnegative matrix with irrational entries whose nonnegative rank over a subfield of $\mathbb{R}$ is different from its nonnegative rank over $\mathbb{R}$. Independently and concurrently with our work [6], Shitov [23] also proposes a rational matrix whose nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ are different.

In the present paper, in order to find a rational matrix that has different nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$, we proceed in two steps. In the first step, we study *restricted* NMFs [14], that is, those factorizations $M' = W \cdot H'$ of a given matrix M' in which the columns of W span the same vector space as the columns of M'. We find irrationality in this setting, constructing a rational matrix M' that has a unique (and irrational) restricted NMF $M' = W \cdot H'$ of inner dimension 5; uniqueness here is understood up to permutation and rescaling of columns of W. In the second step, we transfer this irrationality to our main setting: we construct, based on the matrix M', another matrix M that has a unique (and irrational) NMF $M = W \cdot H$ of inner dimension 5.

For the first step, it has long been known [9] that NMF can be interpreted geometrically as finding a set of vectors (columns of W) inside a unit simplex whose convex hull contains a given set of points (columns of M). It has recently been shown by Gillis and Glineur [14] (see also [7]) that *restricted* NMFs are in one-to-one correspondence with *nested polytopes*: a matrix M' corresponds to a pair of full-dimensional polytopes $\mathcal{R} \subseteq \mathcal{P}$, and a restricted NMF of M' corresponds to a polytope $\mathcal{Q}$ *nested* in between: $\mathcal{R} \subseteq \mathcal{Q} \subseteq \mathcal{P}$. In this paper we find a pair of 3-dimensional polytopes $\mathcal{R} \subseteq \mathcal{P}$ with rational vertices such that there is only one 5-vertex polytope $\mathcal{Q}$ with $\mathcal{R} \subseteq \mathcal{Q} \subseteq \mathcal{P}$, and the vertices of this polytope $\mathcal{Q}$ have irrational coordinates: $\mathcal{R}$ and $\mathcal{P}$ are chosen so as to impose quadratic constraints on the coordinates of the vertices of $\mathcal{Q}$. This gives us a rational matrix M' that has a unique (and irrational) *restricted* NMF $M' = W \cdot H'$ of inner dimension 5.

For the second step, if we knew that the factorization $M' = W \cdot H'$ were unique among *all* NMFs of the same inner dimension, we would be done. This, however, requires ruling out several classes of other hypothetical (nonrestricted) factorizations of the matrix.

Towards this goal, one might want to take advantage of the work on uniqueness properties of NMF, studied, for instance, by Thomas [26], Laurberg et al. [17], and Gillis [12], or on the topology of the set of all NMFs (see Mond, Smith, and van Straten [20]). Here we pursue a different strategy. We show that for a larger matrix $M = \begin{pmatrix} M' & W_\varepsilon \end{pmatrix}$, where W_ε is a nonnegative rational matrix which is entrywise close to W, the only NMF (restricted or otherwise) of the same inner dimension has the same left factor W—thus extending the uniqueness property to the *nonrestricted* setting.

The guiding idea behind our extending M' to M is that by including all columns of W in the set of columns of M, we can exclude certain "undesirable" factorizations, thereby ensuring that M has no rational NMF. We show this by a constraint propagation argument. Unfortunately for this construction, the matrix W itself has irrational entries. However, we show that we can instead take any nonnegative *rational* matrix W_ε within a sufficiently small neighborhood of W, and the undesirable factorizations will still be excluded. In the text we describe such a neighborhood explicitly and pick a specific rational matrix W_ε from it, thus obtaining the matrix M of the above form and proving the main result of the paper.

Conceptually, the existence of a suitable matrix W_ε can be understood in terms of *upper semicontinuity* of the nonnegative rank over $\mathbb{R}$, proved by Bocci, Carlini, and Rapallo [4]. By this property, if a matrix M has nonnegative rank r over $\mathbb{R}$, then all nonnegative matrices in a sufficiently small neighborhood of M have nonnegative rank r or greater (over $\mathbb{R}$). In the same manner, our proof extends the nonexistence of undesirable factorizations from the matrix W to W_ε.

From the computational perspective, nonnegative rank (over $\mathbb{R}$ as well as over $\mathbb{Q}$) is a nontrivial quantity to compute. The usual rank of a matrix M is greater than or equal to r if and only if M has an $r \times r$ submatrix of rank r. The same property does not hold for nonnegative rank. This follows from a construction by Moitra [19] of a family of matrices, indexed by $r, n \in \mathbb{N}$, respectively having size $3rn \times 3rn$ and nonnegative rank at least $4r$, but no $(n-1) \times 3rn$ submatrix of nonnegative rank greater than $3r$. A strengthening of this result can be found in Eggermont, Horobet, and Kubjas [11]; this paper, in fact, studies the set of matrices of nonnegative rank at most 3 and looks into the properties of the boundary of this set.

Deciding whether a given matrix has nonnegative rank at most r is a computationally hard problem, known to be NP-hard due to a result by Vavasis [27]. The problem is easily seen to be reducible to the decision problem for the existential theory of real closed fields and therefore belongs to PSPACE (see, e.g., [5]). Beyond this generic upper bound, the problem has been attacked from many different angles. Here we highlight the results of Arora et al. [2], who identified several variants of the problem that are efficiently solvable, and Moitra [19], who found semialgebraic descriptions of the sets of matrices of nonnegative rank at most r in which the number of variables is $O(r^2)$. However, it remains an open question [27] whether or not the set $\{(M, r)\colon \text{the nonnegative rank of } M \text{ is} \le r\}$ belongs to NP; our solution to the Cohen–Rothblum problem does not exclude either possibility (even though it does rule out a hypothetical "simple" argument for membership in NP, wherein a certificate is an NMF with rational entries of small bit size).

2. Preliminaries.

For any ordered field $\mathbb{F}$, we denote by $\mathbb{F}_+$ the set of all its nonnegative elements. For any vector v, we write v_i for its ith entry. A vector of real numbers v is called *pseudostochastic* if its entries sum up to one. A pseudostochastic vector v is called *stochastic* if its entries are nonnegative.

For any matrix M, we write $M_{i,:}$ for its ith row, $M_{:,j}$ for its jth column, and $M_{i,j}$ for its (i, j)th entry. A matrix is called *nonnegative* if all its entries are nonnegative, it is called *rational* if all its entries are rational, and it is called *zero* if all its entries are zero. A nonnegative matrix is *stochastic* if its columns are stochastic.

2.1. Nonnegative rank.

Let $\mathbb{F}$ be an ordered field, such as the reals $\mathbb{R}$ or the rationals $\mathbb{Q}$. Given a nonnegative matrix $M \in \mathbb{F}_+^{n\times m}$, a *nonnegative matrix factorization (NMF) over* $\mathbb{F}$ of M is any representation of the form $M = W \cdot H$, where $W \in \mathbb{F}_+^{n\times d}$ and $H \in \mathbb{F}_+^{d\times m}$ are nonnegative matrices. We refer to d as the *inner dimension* of the NMF, and hence refer to

NMF $M = W \cdot H$ as being *d-dimensional.* The *nonnegative rank over* $\mathbb{F}$ of M is the smallest nonnegative integer d such that there exists a d-dimensional NMF over $\mathbb{F}$ of M. We may equivalently characterize [9] the nonnegative rank over $\mathbb{F}$ of M as the smallest number of rank-1 matrices in $\mathbb{F}_+^{n\times m}$ such that M is equal to their sum. The nonnegative rank over $\mathbb{R}$ will henceforth simply be called nonnegative rank. For any nonnegative matrix $M \in \mathbb{R}_+^{n\times m}$, it is easy to see that $\mathrm{rank}(M) \le \mathrm{rank}_+(M) \le \min\{n, m\}$, where $\mathrm{rank}(M)$ and $\mathrm{rank}_+(M)$ denote the rank and the nonnegative rank, respectively.

Given a nonzero matrix $M \in \mathbb{F}_+^{n\times m}$, by removing the zero columns of M and dividing each remaining column by the sum of its elements, we obtain a stochastic matrix with equal nonnegative rank. Similarly, if $M = W \cdot H$, then after removing the zero columns in W and multiplying with a suitable diagonal matrix D, we get $M = W \cdot H = WD \cdot D^{-1}H$, where WD is stochastic. If M is stochastic, then (writing $\mathbf{1}$ for a row vector of ones) we have

$$\mathbf{1} = \mathbf{1}M = \mathbf{1}WD \cdot D^{-1}H = \mathbf{1}D^{-1}H,$$

and hence $D^{-1}H$ is stochastic as well. Thus, without loss of generality one can consider NMFs $M = W \cdot H$ in which M, W, and H are all stochastic matrices [9, Theorem 3.2]. In such a case, we will call the factorization $M = W \cdot H$ *stochastic.*

2.2. Nested polygons in the plane.

In this paper all polygons are assumed to be convex. Given two polygons in the plane, $\mathcal{R} \subseteq \mathcal{P} \subseteq \mathbb{R}^2$, a polygon $\mathcal{Q}$ is said to be *nested between* $\mathcal{R}$ *and* $\mathcal{P}$ if $\mathcal{R} \subseteq \mathcal{Q} \subseteq \mathcal{P}$. Such a polygon is said to be *minimal* if it has the minimum number of vertices among all polygons nested between $\mathcal{R}$ and $\mathcal{P}$. In this section we recall from [1] a standardized form for minimal nested polygons, which will play an important role in the subsequent development.

Fix two polygons $\mathcal{R}$ and $\mathcal{P}$, with $\mathcal{R} \subseteq \mathcal{P}$. A *supporting line segment* is a directed line segment uv such that, first, the endpoints u and v lie on the boundary of the outer polygon $\mathcal{P}$ and, second, the inner polygon $\mathcal{R}$ touches uv and lies to the left of uv. A nested polygon with vertices $v_1, \ldots, v_k$, listed in counterclockwise order, is said to be *supporting* if the directed line segments $v_1v_2, v_2v_3, \ldots, v_{k-1}v_k$ are all supporting. (Note that the directed line segment v_kv_1 need not be supporting.) Such a polygon is uniquely determined by the vertex v_1 (see [1, section 2]) and is henceforth denoted by $\mathcal{S}_{v_1}$. It is shown in [1] that some supporting polygon is also minimal. More specifically, from [1, Lemma 4] we have the following lemma.

Lemma 2.1. *Consider a minimal nested polygon with vertices* $v_1, \ldots, v_k$*, listed in counterclockwise order, where* v_1 *lies on the boundary of* $\mathcal{P}$*. The supporting polygon* $\mathcal{S}_{v_1}$ *is also minimal.*

We will need the following elementary fact of linear algebra in connection with subsequent applications of Lemma 2.1. Let $v_1 = (x_1, y_1)$, $v_2 = (x_2, y_2)$, and $v_3 = (x_3, y_3)$ be three distinct points in the plane, and consider the determinant

$$\Delta = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}.$$

Then $\Delta = 0$ if and only if v_1, v_2, and v_3 belong to some common line, and $\Delta > 0$ if and only if the list of vertices v_1, v_2, v_3 describes a triangle with counterclockwise orientation.

3. Main result. We show that the nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ are, in general, different.

Theorem 3.1. *Let* $M = \begin{pmatrix} M' & W_\varepsilon \end{pmatrix} \in \mathbb{Q}_+^{6\times 11}$, *where*

$$M' = \begin{pmatrix} \frac{5}{44} & \frac{5}{11} & \frac{85}{121} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{11} & \frac{3}{11} & \frac{7}{33} \\ \frac{1}{11} & \frac{1}{44} & \frac{2}{121} & \frac{1}{44} & \frac{15}{88} & \frac{17}{88} \\ \frac{1}{44} & \frac{1}{44} & \frac{8}{121} & \frac{1}{44} & \frac{19}{88} & \frac{5}{24} \\ \frac{3}{11} & \frac{3}{11} & \frac{12}{121} & \frac{8}{11} & \frac{2}{11} & \frac{2}{33} \\ \frac{1}{2} & \frac{5}{22} & \frac{14}{121} & \frac{1}{22} & \frac{7}{44} & \frac{43}{132} \end{pmatrix} \in \mathbb{Q}_+^{6\times 6},$$

$$W_\varepsilon = \begin{pmatrix} 0 & \frac{133}{165} & \frac{640}{2233} & 0 & 0 \\ \frac{1}{111540} & 0 & 0 & \frac{17209}{58047} & \frac{997}{5082} \\ \frac{114721}{892320} & \frac{1}{146850} & \frac{17}{506} & \frac{385}{1759} & \frac{2921}{203280} \\ \frac{47}{1248} & \frac{413}{5874} & \frac{1}{102718} & \frac{2915}{10554} & \frac{4381}{203280} \\ \frac{36}{169} & \frac{22}{267} & \frac{18674}{51359} & \frac{1}{116094} & \frac{3252}{4235} \\ \frac{276953}{446160} & \frac{1009}{24475} & \frac{16239}{51359} & \frac{1100}{5277} & \frac{1}{101640} \end{pmatrix} \in \mathbb{Q}_+^{6\times 5}.$$

The nonnegative rank of M over $\mathbb{R}$ is 5*. The nonnegative rank of M over $\mathbb{Q}$ is* 6*.*

The rest of this paper is devoted to the proof of Theorem 3.1.

The matrix M is stochastic. The matrix M' has a stochastic 5-dimensional NMF $M' = W \cdot H'$ with W, H' as follows:

$$W = \begin{pmatrix} 0 & \frac{5}{7} + \frac{5\sqrt{2}}{77} & \frac{15+5\sqrt{2}}{77} & 0 & 0 \\ 0 & 0 & 0 & \frac{20+2\sqrt{2}}{77} & \frac{48-8\sqrt{2}}{187} \\ \frac{\sqrt{2}}{11} & 0 & \frac{4-\sqrt{2}}{77} & \frac{3}{14} + \frac{\sqrt{2}}{308} & \frac{14-8\sqrt{2}}{187} \\ \frac{-1+\sqrt{2}}{11} & \frac{4+\sqrt{2}}{77} & 0 & \frac{39}{154} + \frac{5\sqrt{2}}{308} & \frac{21-12\sqrt{2}}{187} \\ \frac{8-4\sqrt{2}}{11} & \frac{12-4\sqrt{2}}{77} & \frac{4}{11} & 0 & \frac{104+28\sqrt{2}}{187} \\ \frac{4+2\sqrt{2}}{11} & \frac{6-2\sqrt{2}}{77} & \frac{30-4\sqrt{2}}{77} & \frac{3}{11} - \frac{\sqrt{2}}{22} & 0 \end{pmatrix}, \tag{1}$$

$$H' = \begin{pmatrix} \frac{1+\sqrt{2}}{4} & 0 & \frac{\sqrt{2}}{11} & \frac{1}{4} - \frac{\sqrt{2}}{8} & 0 & \frac{1}{6} + \frac{\sqrt{2}}{12} \\ 0 & \frac{1}{2} - \frac{\sqrt{2}}{8} & 1 - \frac{\sqrt{2}}{11} & 0 & 0 & 0 \\ \frac{3-\sqrt{2}}{4} & \frac{1}{2} + \frac{\sqrt{2}}{8} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{21}{34} + \frac{7\sqrt{2}}{68} & \frac{5}{6} - \frac{\sqrt{2}}{12} \\ 0 & 0 & 0 & \frac{3}{4} + \frac{\sqrt{2}}{8} & \frac{13}{34} - \frac{7\sqrt{2}}{68} & 0 \end{pmatrix}.$$

The matrix W_ε has a stochastic 5-dimensional NMF $W_\varepsilon = W \cdot H_\varepsilon$ with H_ε as follows:

$$\begin{pmatrix} \frac{30419}{40560} + \frac{28679\sqrt{2}}{162240} & \frac{-2728}{46725} + \frac{5791\sqrt{2}}{140175} & \frac{2741}{98049} - \frac{642\sqrt{2}}{32683} & \frac{-689}{10554} + \frac{15595\sqrt{2}}{337728} & \frac{389}{1848} - \frac{5501\sqrt{2}}{36960} \\ 0 & \frac{163318}{140175} - \frac{7277\sqrt{2}}{62300} & \frac{5958}{32683} - \frac{50543\sqrt{2}}{392196} & 0 & 0 \\ 0 & \frac{-2137}{20025} + \frac{6047\sqrt{2}}{80100} & \frac{11062}{14007} + \frac{8321\sqrt{2}}{56028} & 0 & 0 \\ \frac{7443}{8840} - \frac{51313\sqrt{2}}{86190} & 0 & 0 & \frac{148897}{179418} + \frac{172627\sqrt{2}}{1435344} & \frac{-1741}{26180} + \frac{1847\sqrt{2}}{39270} \\ \frac{-408157}{689520} + \frac{1154473\sqrt{2}}{2758080} & 0 & 0 & \frac{7039}{29903} - \frac{318541\sqrt{2}}{1913792} & \frac{134461}{157080} + \frac{1163\sqrt{2}}{11424} \end{pmatrix}.$$

Hence, the matrix M has a stochastic 5-dimensional NMF as follows:

$$M = W \cdot \begin{pmatrix} H' & H_\varepsilon \end{pmatrix}. \tag{2}$$

We refer the reader to [30] for a Maple worksheet with calculations of the paper.

Remark 3.2. The columns of M and W span the same vector space. It follows that the *restricted* nonnegative ranks of M over $\mathbb{R}$ and $\mathbb{Q}$ are 5 and 6, respectively. In fact, the authors of this paper previously exhibited a rational nonnegative matrix whose restricted nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ differ [7].

We fix the matrices $M, M', W_\varepsilon, W, H', H_\varepsilon$ for the remainder of the paper.

3.1. Types of factorizations.

Let $M = L \cdot R$ be a stochastic NMF of inner dimension at most 5. (As argued in section 2.1, without loss of generality we may consider only stochastic NMFs of M.) Let us introduce the following notation:

- k is the number of columns in L whose first and second coordinates are 0,
- k_1 is the number of columns in L whose first coordinate is strictly positive and second coordinate is 0, and
- k_2 is the number of columns in L whose second coordinate is strictly positive and first coordinate is 0.

Clearly, the factorization $M = L \cdot R$ corresponds to representing each column of M as a convex combination of the columns of L, with the coefficients of the convex combination specified by the entries of R. As L has at most five columns,

$$k + k_1 + k_2 \leq 5. \tag{3}$$

Since the columns $M_{:,1}, M_{:,2}, M_{:,3}$ are linearly independent, the matrix L has at least three columns whose second coordinate is 0. Likewise, since the columns $M_{:,4}, M_{:,5}, M_{:,6}$ are linearly independent, L has at least three columns whose first coordinate is 0. That is,

$$k + k_1 \geq 3 \quad \text{and} \quad k + k_2 \geq 3. \tag{4}$$

Together with (3), this implies that $2k \geq 6 - k_1 - k_2 \geq 1 + k$, and therefore $k \geq 1$.

The columns $M_{:,1}, M_{:,2}, M_{:,3}$ have first coordinate strictly positive and second coordinate 0, while the columns $M_{:,4}, M_{:,5}, M_{:,6}$ have second coordinate strictly positive and first coordinate 0. Therefore, in order for these columns to be covered by columns of L, we need to have

$$k_1 \geq 1 \quad \text{and} \quad k_2 \geq 1. \tag{5}$$

$$
\overset{\text{type 1}}{\begin{pmatrix} 0 & + & + & 0 & 0 \\ 0 & 0 & 0 & + & + \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}}
\qquad
\overset{\text{type 2}}{\begin{pmatrix} 0 & 0 & + & \cdot & \cdot \\ 0 & 0 & 0 & + & + \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}}
\qquad
\overset{\text{type 3}}{\begin{pmatrix} 0 & 0 & 0 & + & + \\ 0 & 0 & + & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}}
\qquad
\overset{\text{type 4}}{\begin{pmatrix} + & 0 & 0 & 0 & 0 \\ 0 & + & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}}
$$

Figure 1. *In any 5-dimensional NMF $M = L \cdot R$, the matrix L matches one of the four patterns above, up to a permutation of its columns. Here $+$ denotes any strictly positive number.*

Together with (3), this implies that $k \le 5 - k_1 - k_2 \le 3$. We conclude that $k \in \{1, 2, 3\}$. More precisely, it is now a consequence of inequalities (3), (4), and (5) that the NMF $M = L \cdot R$ has (at least) one of the following four *types*:

1. $k = 1$, $k_1 = 2$, $k_2 = 2$;
2. $k = 2$, $k_1 = 1$, $k_2 \in \{0, 1, 2\}$;
3. $k = 2$, $k_2 = 1$, $k_1 \in \{0, 1, 2\}$;
4. $k = 3$, $k_1 = 1$, $k_2 = 1$.

These four types are illustrated in Figure 1 for NMFs of inner dimension 5.

In section 4 we prove the following proposition.

Proposition 3.3. *Let M be the matrix from Theorem 3.1 and W the matrix from (1).*
1. *If $M = L \cdot R$ is a type-1 NMF, then $W_{:,1}$ is a column of L, and thus L is not rational.*
2. *The matrix M has no type-2 NMF.*
3. *The matrix M has no type-3 NMF.*
4. *The matrix M has no type-4 NMF.*

Using this proposition, we can prove Theorem 3.1.

Proof of Theorem 3.1. Due to the NMF of M stated in (2), the nonnegative rank of M is at most 5. If there existed an at most 4-dimensional NMF of M, then, as $k + k_1 + k_2 \le 4$, it would have to have type 2 or 3, but those types are excluded by items 2 and 3 of Proposition 3.3. Hence the nonnegative rank of M over $\mathbb{R}$ equals 5.

Since $M = I \cdot M$ (where I denotes the 6×6 identity matrix), the nonnegative rank of M over $\mathbb{Q}$ is at most 6. By Proposition 3.3 there is no 5-dimensional NMF $M = L \cdot R$ with L rational. Hence, the nonnegative rank of M over $\mathbb{Q}$ equals 6. ∎

4. Proof of Proposition 3.3.

It remains to prove Proposition 3.3. To rule out type-4 NMFs, we use constraint propagation in order to prove that the inequalities required for type-4 NMFs are contradictory; see section 4.5. To rule out rational NMFs of types 1, 2, and 3, we employ geometric arguments concerning nested polygons in the plane (see sections 4.2–4.4). These arguments rely on a geometric interpretation of the specific NMF $M = W \cdot \begin{pmatrix} H' & H_\varepsilon \end{pmatrix}$ given by (2). More precisely, we define a polytope $\mathcal{P} \subseteq \mathbb{R}^3$, shown in Figure 2, such that each of the columns of M and W can be associated with a point in $\mathcal{P}$. The points associated with the columns of M lie in the convex hull of those associated with the columns of W (cf. [14]).

4.1. Geometry behind the proof of Proposition 3.3. To set up this geometric connection, observe that the matrix M is stochastic and has rank 4, and hence the columns of M affinely span a 3-dimensional affine subspace $\mathcal{V} \subseteq \mathbb{R}^6$. All vectors in $\mathcal{V}$ are pseudostochastic. The set of stochastic vectors in $\mathcal{V}$ (equivalently, the nonnegative vectors in $\mathcal{V}$) form a 3-dimensional polytope, say $\mathcal{P}' \subseteq \mathcal{V}$. Clearly we have $M_{:,i} \in \mathcal{P}'$ for each $i \in \{1, \dots, 11\}$.

Parameterization. We will now fix a particular parameterization of $\mathcal{V}$ and $\mathcal{P}'$; that is, we define an injective affine function $f : \mathbb{R}^3 \to \mathbb{R}^6$ and a polytope $\mathcal{P} \subseteq \mathbb{R}^3$ such that $f(\mathbb{R}^3) = \mathcal{V}$ and $f(\mathcal{P}) = \mathcal{P}'$. Let $f : \mathbb{R}^3 \to \mathbb{R}^6$ be the function with $f(x) = Cx + d$ for each $x \in \mathbb{R}^3$, where

$$C = \frac{1}{11} \cdot \begin{pmatrix} 0 & 10 & 0 \\ 0 & 0 & 4 \\ -1 & -2 & 1/2 \\ -1 & 0 & 5/2 \\ 4 & 0 & 0 \\ -2 & -8 & -7 \end{pmatrix} \in \mathbb{Q}^{6\times 3} \quad \text{and} \quad d = \frac{1}{11} \cdot \begin{pmatrix} 0 \\ 0 \\ 2 \\ 1 \\ 0 \\ 8 \end{pmatrix} \in \mathbb{Q}^{6\times 1}.$$

Note that the map f is injective.

Defining

$$r_1 = \begin{pmatrix} 3/4 \\ 1/8 \\ 0 \end{pmatrix}, \; r_2 = \begin{pmatrix} 3/4 \\ 1/2 \\ 0 \end{pmatrix}, \; r_3 = \begin{pmatrix} 3/11 \\ 17/22 \\ 0 \end{pmatrix}, \; r_4 = \begin{pmatrix} 2 \\ 0 \\ 1/2 \end{pmatrix}, \; r_5 = \begin{pmatrix} 1/2 \\ 0 \\ 3/4 \end{pmatrix}, \; r_6 = \begin{pmatrix} 1/6 \\ 0 \\ 7/12 \end{pmatrix},$$

we have $f(r_i) = M'_{:,i}$ for each $i \in \{1, 2, \dots, 6\}$, and defining

$$q_1^\varepsilon = \begin{pmatrix} \frac{99}{169} \\ 0 \\ \frac{1}{40560} \end{pmatrix}, \; q_2^\varepsilon = \begin{pmatrix} \frac{121}{534} \\ \frac{133}{150} \\ 0 \end{pmatrix}, \; q_3^\varepsilon = \begin{pmatrix} \frac{9337}{9338} \\ \frac{64}{203} \\ 0 \end{pmatrix}, \; q_4^\varepsilon = \begin{pmatrix} \frac{1}{42216} \\ 0 \\ \frac{17209}{21108} \end{pmatrix}, \; q_5^\varepsilon = \begin{pmatrix} \frac{813}{385} \\ 0 \\ \frac{997}{1848} \end{pmatrix},$$

we have $f(q_i^\varepsilon) = (W_\varepsilon)_{:,i}$ for each $i \in \{1, 2, \dots, 5\}$. Thus, all columns of M lie in the image of f. It follows that $f(\mathbb{R}^3) = \mathcal{V}$.

Let $\mathcal{P}$ be the 3-dimensional polytope defined by $\{\, x \in \mathbb{R}^3 \mid f(x) \geq 0 \,\}$. Then $f(\mathcal{P}) = \mathcal{P}'$. Furthermore, $r_i \in \mathcal{P}$, as $f(r_i) = M'_{:,i} \in \mathcal{P}'$ for all $i \in \{1, 2, \dots, 6\}$. Likewise we have $q_i^\varepsilon \in \mathcal{P}$, as $f(q_i^\varepsilon) = (W_\varepsilon)_{:,i} \in \mathcal{P}'$ for all $i \in \{1, 2, \dots, 5\}$.

Figure 2 visualizes $\mathcal{P}$, which has 6 faces corresponding to the inequalities of the system $Cx + d \geq 0$. In more detail, $\mathcal{P}$ is the intersection of the following half-spaces: $y \geq 0$ (blue), $z \geq 0$ (brown), $-\frac{1}{2}x - y + \frac{1}{4}z + 1 \geq 0$ (green), $-x + \frac{5}{2}z + 1 \geq 0$ (yellow), $x \geq 0$ (pink), $-\frac{1}{4}x - y - \frac{7}{8}z + 1 \geq 0$ (transparent front). The figure also shows the position of the points $r_1, \dots, r_6$ (black dots).[1]

In fact, the columns of W are also in $\mathcal{P}' \subseteq \mathcal{V}$. Indeed, defining

$$q_1^* = \begin{pmatrix} 2 - \sqrt{2} \\ 0 \\ 0 \end{pmatrix}, \; q_2^* = \begin{pmatrix} \frac{3-\sqrt{2}}{7} \\ \frac{11+\sqrt{2}}{14} \\ 0 \end{pmatrix}, \; q_3^* = \begin{pmatrix} 1 \\ \frac{3+\sqrt{2}}{14} \\ 0 \end{pmatrix}, \; q_4^* = \begin{pmatrix} 0 \\ 0 \\ \frac{10+\sqrt{2}}{14} \end{pmatrix}, \; q_5^* = \begin{pmatrix} \frac{26+7\sqrt{2}}{17} \\ 0 \\ \frac{12-2\sqrt{2}}{17} \end{pmatrix},$$

[1]In [7] the authors of the current paper used the same polytope $\mathcal{P}$ and the same points $r_1, \dots, r_6$ (see Figure 2) to prove a related result about the *restricted* nonnegative rank.

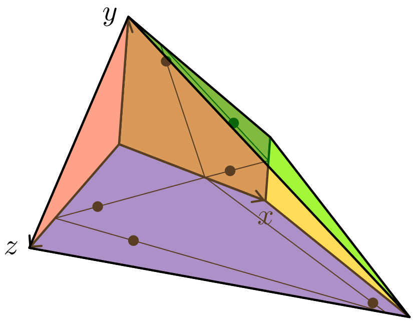

Figure 2. *The two images show orthogonal projections of the 3-dimensional polytope $\mathcal{P}$. The black dots indicate 6 interior points: 3 points (r_1, r_2, r_3) on the brown xy-face, and 3 points (r_4, r_5, r_6) on the blue xz-face. (The images form a stereo pair intended for "parallel-eye" watching: to see the polytope in 3D, look at the left and right projections with your left and right eyes, respectively, at the same time, as described, e.g., in* [25]*.)*

we have $f(q_i^*) = W_{:,i} \in \mathcal{P}'$, and hence $q_i^* \in \mathcal{P}$ for each $i \in \{1, 2, \ldots, 5\}$. That is, in our NMF $M = W \cdot \begin{pmatrix} H' & H_\varepsilon \end{pmatrix}$, the columns of M and the columns of W span the same vector space. Such NMFs are called *restricted* in [14] and [7]. Applying the inverse of the map f columnwise to the NMFs $M' = W \cdot H'$ and $W_\varepsilon = W \cdot H_\varepsilon$, we obtain

$$\begin{aligned} \begin{pmatrix} r_1 & r_2 & r_3 & r_4 & r_5 & r_6 \end{pmatrix} &= \begin{pmatrix} q_1^* & q_2^* & q_3^* & q_4^* & q_5^* \end{pmatrix} \cdot H' \qquad \text{and} \\ \begin{pmatrix} q_1^\varepsilon & q_2^\varepsilon & q_3^\varepsilon & q_4^\varepsilon & q_5^\varepsilon \end{pmatrix} &= \begin{pmatrix} q_1^* & q_2^* & q_3^* & q_4^* & q_5^* \end{pmatrix} \cdot H_\varepsilon \,, \end{aligned} \tag{6}$$

respectively. Recall that the matrix H' is stochastic; hence (6) implies that the points r_i and q_i^ε are contained in the convex hull of the points q_i^*. In Figure 2, points q_1^*, q_2^*, q_3^* are the vertices of the triangle on the brown xy-face, while points q_1^*, q_4^*, q_5^* are the vertices of the triangle on the blue xz-face. The former triangle contains r_1, r_2, r_3, while the latter triangle contains r_4, r_5, r_6. Points $q_1^\varepsilon, \ldots, q_5^\varepsilon$ (not shown in Figure 2) are close to $q_1^*, \ldots, q_5^*$, with $q_2^\varepsilon, q_3^\varepsilon$ lying in the interior of the triangle on the xy-face and $q_1^\varepsilon, q_4^\varepsilon, q_5^\varepsilon$ lying in the interior of the triangle on the xz-face.

It is important to note that when we exclude certain NMFs $M = L \cdot R$ in sections 4.2–4.5, we cannot a priori assume that the columns of L are in $\mathcal{V}$.

Nested polygons. In this subsection, we focus on the two faces of polytope $\mathcal{P}$ that contain the interior points r_1, r_2, r_3 and r_4, r_5, r_6, respectively called $\mathcal{P}_0$ and $\mathcal{P}_1$.

Let us write $\mathcal{V}_0 \subseteq \mathbb{R}^6$ for the affine span of $M_{:,1}, M_{:,2}, M_{:,3}$. We can also characterize $\mathcal{V}_0$ as the image of the xy-plane in $\mathbb{R}^3$ under the map $f : \mathbb{R}^3 \to \mathbb{R}^6$. Indeed, we have $f(r_1) = M_{:,1}$, $f(r_2) = M_{:,2}$, and $f(r_3) = M_{:,3}$. Thus the image of the xy-plane under f is a 2-dimensional affine space that includes $\mathcal{V}_0$ and hence is equal to $\mathcal{V}_0$. Define the polygon $\mathcal{P}_0 \subseteq \mathbb{R}^3$ by $\mathcal{P}_0 = \{(x, y, 0)^\top : (x, y, 0)^\top \in \mathcal{P}\}$. Then f restricts to a bijection between $\mathcal{P}_0$ and the set of nonnegative vectors in $\mathcal{V}_0$. We have the following lemma.

Lemma 4.1. *Let $\mathcal{R}_0 \subseteq \mathcal{P}_0$ be the polygon with vertices r_1, r_2, r_3 (see Figure 3). Write $q_1 = (u, 0, 0)^\top$, where $0 \le u \le 1$. If the supporting polygon $\mathcal{S}_{q_1}$ nested between $\mathcal{R}_0$ and $\mathcal{P}_0$ has three vertices, then $u \ge 2 - \sqrt{2}$.*

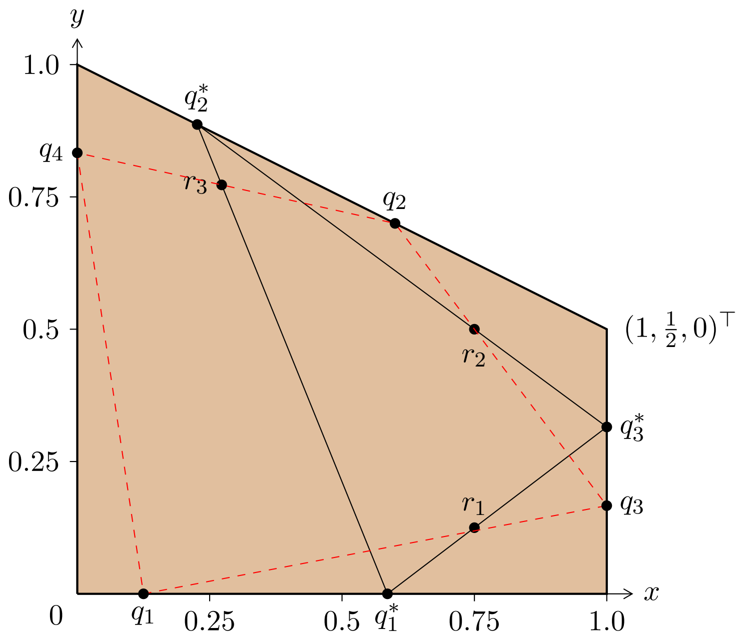

Figure 3. *The outer polygon is $\mathcal{P}_0$ (after identifying the xy-plane in $\mathbb{R}^3$ with $\mathbb{R}^2$). The triangle with solid boundary is the supporting polygon $\mathcal{S}_{q_1^*}$, where $q_1^* = (2-\sqrt{2}, 0, 0)^\top$. The quadrilateral with dashed boundary is the supporting polygon $\mathcal{S}_{q_1}$ for $q_1 = (\frac{1}{8}, 0, 0)^\top$.*

Proof. Assume that $\mathcal{S}_{q_1}$ has three vertices and that $0 \le u \le 2-\sqrt{2}$. It suffices to show that these assumptions imply $u = 2-\sqrt{2}$. Moving counterclockwise, let the vertices of $\mathcal{S}_{q_1}$ be q_1, q_3, and q_2. It follows by elementary geometry that (i) the line segment q_1q_3 passes through r_1 and q_3 lies on the right edge of $\mathcal{P}_0$, and (ii) the line segment q_3q_2 passes through r_2 and q_2 lies on the upper edge of $\mathcal{P}_0$. Figure 3 shows the situations $u = 2-\sqrt{2}$ and $u = \frac{1}{8}$.

Writing $q_3 = (1, \frac{v}{2}, 0)^\top$ and $q_2 = (1-w, \frac{1}{2}+\frac{w}{2}, 0)^\top$, where $0 \le v, w \le 1$, the collinearity conditions (i) and (ii) entail (see section 2.2)

$$\begin{vmatrix} u & 0 & 1 \\ 1 & \frac{v}{2} & 1 \\ \frac{3}{4} & \frac{1}{8} & 1 \end{vmatrix} = \frac{1}{2}uv - \frac{1}{8}u - \frac{3}{8}v + \frac{1}{8} = 0 \quad \text{and} \tag{7}$$

$$\begin{vmatrix} 1 & \frac{v}{2} & 1 \\ 1-w & \frac{1}{2}+\frac{w}{2} & 1 \\ \frac{3}{4} & \frac{1}{2} & 1 \end{vmatrix} = \frac{1}{2}vw - \frac{1}{8}v - \frac{3}{8}w + \frac{1}{8} = 0\,. \tag{8}$$

The assumption that $\mathcal{S}_{q_1}$ is the triangle $\triangle q_1q_3q_2$ entails that vertices q_2, q_1, r_3 are in counterclockwise order. This implies

$$\begin{vmatrix} 1-w & \frac{1}{2}+\frac{w}{2} & 1 \\ u & 0 & 1 \\ \frac{3}{11} & \frac{17}{22} & 1 \end{vmatrix} = -\frac{1}{2}wu + \frac{10}{11}w + \frac{3}{11}u - \frac{7}{11} \ge 0. \tag{9}$$

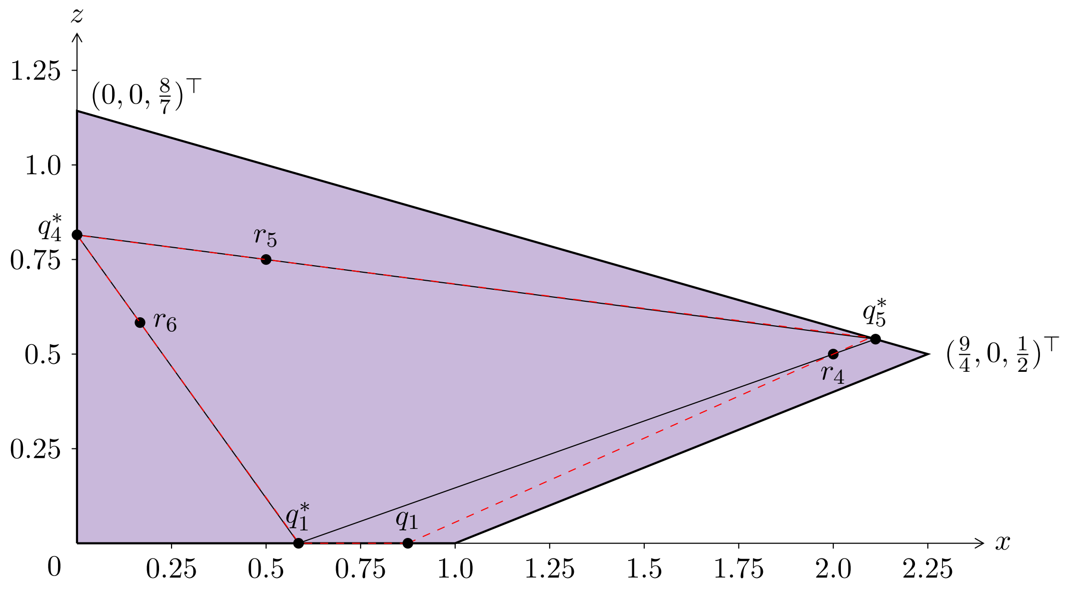

Figure 4. *The outer polygon is $\mathcal{P}_1$ (after identifying the xz-plane in $\mathbb{R}^3$ with $\mathbb{R}^2$). The triangle with solid boundary is the supporting polygon $\mathcal{S}_{q_1^*}$, where $q_1^* = (2-\sqrt{2}, 0, 0)^\top$. The quadrilateral with dashed boundary is the supporting polygon $\mathcal{S}_{q_1}$ for $q_1 = (\frac{7}{8}, 0, 0)^\top$.*

We use (7) and (8) to eliminate variables v, w from inequality (9), obtaining

$$\frac{15}{22(8u-5)} \cdot (u^2 - 4u + 2) \geq 0.$$

The only solution with $0 \leq u \leq 2-\sqrt{2}$ is $u = 2-\sqrt{2}$. ∎

Let us write $\mathcal{V}_1 \subseteq \mathbb{R}^6$ for the affine span of $M_{:,4}, M_{:,5}, M_{:,6}$. We can also characterize $\mathcal{V}_1$ as the image of the xz-plane in $\mathbb{R}^3$ under the map $f : \mathbb{R}^3 \to \mathbb{R}^6$. Indeed, we have $f(r_4) = M_{:,4}$, $f(r_5) = M_{:,5}$, and $f(r_6) = M_{:,6}$. Thus the image of the xz-plane under f is a 2-dimensional affine space that includes $\mathcal{V}_1$ and hence is equal to $\mathcal{V}_1$. Define the polygon $\mathcal{P}_1 \subseteq \mathbb{R}^3$ by $\mathcal{P}_1 = \{(x, 0, z)^\top : (x, 0, z)^\top \in \mathcal{P}\}$. Then f restricts to a bijection between $\mathcal{P}_1$ and the set of nonnegative vectors in $\mathcal{V}_1$. We have the following lemma.

Lemma 4.2. *Let $\mathcal{R}_1 \subseteq \mathcal{P}_1$ be the polygon with vertices r_4, r_5, r_6 (see Figure 4). Write $q_1 = (u, 0, 0)^\top$, where $0 \leq u \leq 1$. If the supporting polygon $\mathcal{S}_{q_1}$ nested between $\mathcal{R}_1$ and $\mathcal{P}_1$ has three vertices, then $u \leq 2-\sqrt{2}$.*

Proof. Assume that $\mathcal{S}_{q_1}$ has three vertices and that $2-\sqrt{2} \leq u \leq 1$. It suffices to show that these assumptions imply $u = 2-\sqrt{2}$. Moving counterclockwise, let the vertices of $\mathcal{S}_{q_1}$ be q_1, q_5, and q_4. It follows by elementary geometry that (i) the line segment q_1q_5 passes through r_4 and q_5 lies on the upper edge of $\mathcal{P}_1$, and (ii) the line segment q_5q_4 passes through r_5 and q_4 lies on the left edge of $\mathcal{P}_1$. Figure 4 shows the situations $u = 2-\sqrt{2}$ and $u = \frac{7}{8}$.

Writing $q_5 = (\frac{9-9v}{4}, 0, \frac{7+9v}{14})^\top$ and $q_4 = (0, 0, \frac{8-8w}{7})^\top$, where $0 \leq v, w \leq 1$, the collinearity conditions (i) and (ii) entail (see section 2.2)

$$\begin{vmatrix} u & 0 & 1 \\ \frac{9-9v}{4} & \frac{7+9v}{14} & 1 \\ 2 & \frac{1}{2} & 1 \end{vmatrix} = \frac{9}{14}uv - \frac{135}{56}v + \frac{1}{8} \qquad = 0 \qquad \text{and} \tag{10}$$

$$\begin{vmatrix} \frac{9-9v}{4} & \frac{7+9v}{14} & 1 \\ 0 & \frac{8-8w}{7} & 1 \\ \frac{1}{2} & \frac{3}{4} & 1 \end{vmatrix} = \frac{18}{7}vw - \frac{9}{16}v - 2w + \frac{9}{16} \ = 0. \tag{11}$$

The assumption that $\mathcal{S}_{q_1}$ is the triangle $\triangle q_1 q_5 q_4$ entails that vertices q_4, q_1, r_6 are in counter-clockwise order. This implies

$$\begin{vmatrix} 0 & \frac{8-8w}{7} & 1 \\ u & 0 & 1 \\ \frac{1}{6} & \frac{7}{12} & 1 \end{vmatrix} = \frac{8}{7}wu - \frac{4}{21}w - \frac{47}{84}u + \frac{4}{21} \geq 0. \tag{12}$$

We use (10) and (11) to eliminate variables v, w from the inequality (12), obtaining

$$\frac{-10}{21(2u-7)} \cdot (u^2 - 4u + 2) \quad \geq 0.$$

The only solution with $2 - \sqrt{2} \leq u \leq 1$ is $u = 2 - \sqrt{2}$. ■

4.2. Type 1. In this section we prove Proposition 3.3(1), implying that any type-1 NMF of M requires irrational numbers (our argument will, in fact, depend only on the matrix M' and not on W_ε). Consider a type-1 NMF $M = L \cdot R$, i.e., such that $k = 1$ and $k_1 = k_2 = 2$. After a suitable permutation of its columns, L matches the pattern

$$L = \begin{pmatrix} 0 & + & + & 0 & 0 \\ 0 & 0 & 0 & + & + \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

where $+$ denotes any strictly positive number. It follows from the zero pattern of M that $M_{:,1}, M_{:,2}, M_{:,3}$ all lie in the convex hull of $L_{:,1}, L_{:,2}, L_{:,3}$, and $M_{:,4}, M_{:,5}, M_{:,6}$ all lie in the convex hull of $L_{:,1}, L_{:,4}, L_{:,5}$. Equivalently, there exist stochastic matrices $R_0, R_1 \in \mathbb{R}_+^{3\times 3}$ such that

$$\begin{aligned} \begin{pmatrix} M_{:,1} & M_{:,2} & M_{:,3} \end{pmatrix} &= \begin{pmatrix} L_{:,1} & L_{:,2} & L_{:,3} \end{pmatrix} \cdot R_0 \qquad \text{and} \\ \begin{pmatrix} M_{:,4} & M_{:,5} & M_{:,6} \end{pmatrix} &= \begin{pmatrix} L_{:,1} & L_{:,4} & L_{:,5} \end{pmatrix} \cdot R_1 \,. \end{aligned} \tag{13}$$

Consider the polygon $\mathcal{P}_0 \subseteq \mathbb{R}^3$ and the affine space $\mathcal{V}_0 \subseteq \mathbb{R}^6$ from section 4.1. The affine span of $L_{:,1}, L_{:,2}, L_{:,3}$ includes $\mathcal{V}_0$ and has dimension at most 2, and hence is equal to $\mathcal{V}_0$. In particular, $L_{:,1}, L_{:,2}, L_{:,3}$ must all lie in $\mathcal{V}_0$. Since $L_{:,1}, L_{:,2}, L_{:,3}$ are, moreover, nonnegative, there are uniquely defined points $q_1, q_2, q_3 \in \mathcal{P}_0$ such that $f(q_i) = L_{:,i}$ for $i \in \{1, 2, 3\}$. Applying the inverse of the map f columnwise to (13), we obtain

$$\begin{pmatrix} r_1 & r_2 & r_3 \end{pmatrix} = \begin{pmatrix} q_1 & q_2 & q_3 \end{pmatrix} \cdot R_0 ,$$

so the convex hull of q_1, q_2, q_3 includes r_1, r_2, r_3. In other words, triangle $\triangle q_1 q_2 q_3$ is nested between $\triangle r_1 r_2 r_3$ and polygon $\mathcal{P}_0$. Since $L_{:,1}$ has 0 in its first two coordinates, by inspecting the definition of the map f we see that $q_1 = (u, 0, 0)^\top$ for some $u \in \mathbb{R}$. By Lemma 2.1 it follows that the supporting polygon $\mathcal{S}_{q_1}$ has three vertices. Hence Lemma 4.1 implies $u \geq 2 - \sqrt{2}$.

Considering the polygon $\mathcal{P}_1$ from section 4.1, we have $q_1 \in \mathcal{P}_1$ (recall that $f(q_1) = L_{:,1}$). Arguing as in the case of $\mathcal{P}_0$, there are uniquely defined points $q_4, q_5 \in \mathcal{P}_1$ such that $f(q_i) = L_{:,i}$ for $i \in \{4, 5\}$. Similarly as before, triangle $\triangle q_1 q_4 q_5$ is nested between $\triangle r_4 r_5 r_6$ and $\mathcal{P}_1$. Then Lemmas 2.1 and 4.2 imply $u \leq 2 - \sqrt{2}$, and thus $q_1 = (2 - \sqrt{2}, 0, 0)^\top = q_1^*$. Hence

$$L_{:,1} = f(q_1) = f(q_1^*) = W_{:,1}.$$

Proposition 3.3(1) follows.

We remark that this argument can be strengthened to show that any type-1 NMF of M coincides with the one given in (2), up to a permutation of the columns of W and the rows of $\begin{pmatrix} H' & H_\varepsilon \end{pmatrix}$; see Appendix A.

4.3. Type 2. In this section we exclude type-2 NMFs, i.e., we prove Proposition 3.3(2). Towards a contradiction, suppose there is a stochastic and at most 5-dimensional NMF $M = L \cdot R$ with $k = 2$ and $k_1 = 1$. Without loss of generality, the first three columns of L match the following pattern:

$$\begin{array}{ccc} L_{:,1} & L_{:,2} & L_{:,3} \\ \end{array}$$
$$\begin{pmatrix} 0 & 0 & + \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix},$$

and the remaining columns have a strictly positive second coordinate. It follows from the zero pattern of M that $M_{:,1}, M_{:,2}, M_{:,3}$ all lie in the convex hull of $L_{:,1}, L_{:,2}, L_{:,3}$.

Consider again the polygon $\mathcal{P}_0 \subseteq \mathbb{R}^3$. For the purposes of the following argument, $\mathcal{P}_0$ is visualized on the left in Figure 5. Reasoning analogously to section 4.2, there are unique points $q_1, q_2, q_3 \in \mathcal{P}_0$ with $f(q_i) = L_{:,i}$ for $i \in \{1, 2, 3\}$, and the convex hull of q_1, q_2, q_3 includes r_1, r_2, r_3. Since $L_{:,1}$ and $L_{:,2}$ have 0 in their first two rows, inspecting the definition of the map f, we see that q_1 and q_2 lie on the x-axis in $\mathbb{R}^3$. Thus, writing $\hat{q}_1 = (0, 0, 0)^\top$ and $\hat{q}_2 = (1, 0, 0)^\top$, triangle $\triangle \hat{q}_1 \hat{q}_2 q_3$ includes triangle $\triangle q_1 q_2 q_3$ and hence also contains the points r_1, r_2, r_3. But clearly there is no point $q_3 \in \mathcal{P}_0$ such that $\triangle \hat{q}_1 \hat{q}_2 q_3$ includes both r_2 and r_3 (see, e.g., Figure 5, left), which is a contradiction. Thus we have proved Proposition 3.3(2).

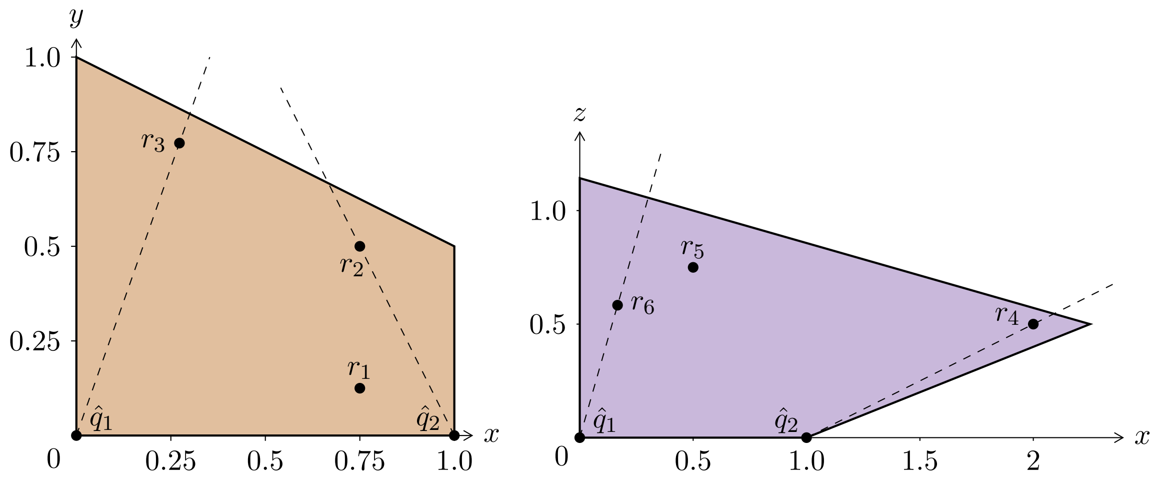

Figure 5. *Left: there is no point q_3 in the quadrilateral $\mathcal{P}_0$ such that $\triangle \hat{q}_1\hat{q}_2q_3$ includes both r_2 and r_3. Right: there is no point q_3 in the quadrilateral $\mathcal{P}_1$ such that $\triangle \hat{q}_1\hat{q}_2q_3$ includes both r_4 and r_6.*

4.4. Type 3. In this section we exclude type-3 NMFs, i.e., we prove Proposition 3.3(3). The reasoning is entirely analogous to section 4.3. Towards a contradiction, suppose there is a stochastic and at most 5-dimensional NMF $M = L \cdot R$ with $k = 2$ and $k_2 = 1$. Consider again the polygon $\mathcal{P}_1 \subseteq \mathbb{R}^3$. For the purposes of the following argument, $\mathcal{P}_1$ is visualized on the right in Figure 5. Analogously to section 4.3, there are points $q_1, q_2, q_3 \in \mathcal{P}_1$ whose convex hull includes r_4, r_5, r_6, and q_1 and q_2 lie on the x-axis in $\mathbb{R}^3$. Thus, writing $\hat{q}_1 = (0,0,0)^\top$ and $\hat{q}_2 = (1,0,0)^\top$, triangle $\triangle \hat{q}_1\hat{q}_2q_3$ includes the points r_4, r_5, r_6. But clearly there is no point $q_3 \in \mathcal{P}_1$ such that $\triangle \hat{q}_1\hat{q}_2q_3$ includes both r_4 and r_6 (see, e.g., Figure 5, right), which is a contradiction. Thus we have proved Proposition 3.3(3).

4.5. Type 4. In this section we exclude type-4 NMFs, i.e., we prove Proposition 3.3(4). In fact, sections 4.2–4.4 prove the stronger result that there is no rational NMF of types 1, 2, 3 for the matrix M' alone. Here we spell out the role of W_ε, effectively explaining why the matrix $M = \begin{pmatrix} M' & W_\varepsilon \end{pmatrix}$ is defined the way it is.

Observe that adding to M' new columns from the convex hull of the columns of W shrinks the set of possible nonnegative factorizations. Given this, our goal is to find a matrix satisfying the following desiderata:

- its entries are rational,
- its columns belong to the convex hull of the columns of W, and
- it has no type-4 NMF.

The first two items ensure that M, while being rational, admits a nonnegative factorization with left factor W, ensuring that the nonnegative rank of M over $\mathbb{R}$ is (at most) 5. The third condition, combined with the arguments from sections 4.2–4.4, ensures that the nonnegative rank of M over $\mathbb{Q}$ is 6.

While the matrix W manifestly fails the first desideratum, it satisfies the second and third as follows.

Claim 4.3. *The matrix W and, therefore, the matrix $\overline{M} = \begin{pmatrix} M' & W \end{pmatrix}$ have no type-4 NMF.*

$$\widetilde{W} = \begin{array}{cc} & \begin{array}{ccccc} \widetilde{W}_{:,1} & \widetilde{W}_{:,2} & \widetilde{W}_{:,3} & \widetilde{W}_{:,4} & \widetilde{W}_{:,5} \end{array} \\ \begin{array}{c} \widetilde{W}_{1,:} \\ \widetilde{W}_{2,:} \\ \widetilde{W}_{3,:} \\ \widetilde{W}_{4,:} \\ \widetilde{W}_{5,:} \\ \widetilde{W}_{6,:} \end{array} & \begin{pmatrix} 0 & 0.8 \leq \cdot & 0.286 \leq \cdot \leq 0.287 & 0 & 0 \\ \cdot \leq \varepsilon & 0 & 0 & 0.29 \leq \cdot & 0.196 \leq \cdot \\ & \cdot \leq \varepsilon & 0.0335 \leq \cdot & 0.21 \leq \cdot & \cdot \leq 0.015 \\ & 0.07 \leq \cdot & \cdot \leq \varepsilon & 0.27 \leq \cdot & \cdot \leq 0.022 \\ & & & \cdot \leq \varepsilon & 0.767 \leq \cdot \\ 0.62 \leq \cdot & & \cdot \leq 0.32 & \cdot \leq 0.21 & \cdot \leq \varepsilon \end{pmatrix} \end{array}$$

Figure 6. *Entrywise constraints, where* $\varepsilon = 10^{-5}$.

$$W_\varepsilon \approx \begin{pmatrix} 0 & 0.81 & 0.2866 & 0 & 0 \\ 0.9 \cdot 10^{-5} & 0 & 0 & 0.296 & 0.1962 \\ 0.1 & 0.7 \cdot 10^{-5} & 0.03360 & 0.219 & 0.0144 \\ 0.04 & 0.0703 & 0.97 \cdot 10^{-5} & 0.276 & 0.0216 \\ 0.2 & 0.08 & 0.4 & 0.9 \cdot 10^{-5} & 0.7679 \\ 0.621 & 0.04 & 0.316 & 0.208 & 0.98 \cdot 10^{-5} \end{pmatrix}$$

Figure 7. *Matrix* W_ε *with entries rounded off.*

This reasoning motivates the main technical result of this section, which is a strengthening of Claim 4.3 showing that no matrix in a suitably small neighborhood of W admits a type-4 NMF.

Lemma 4.4. *For all stochastic matrices* $\widetilde{W} \in \mathbb{R}_+^{6\times 5}$ *satisfying the entrywise constraints given in Figure 6, there exists no type-*4 *NMF* $\widetilde{W} = L \cdot R$.

In particular, the constraints of Lemma 4.4, and in fact all three desiderata, are satisfied by the matrix W_ε from Theorem 3.1; see Figure 7. Therefore, the matrix $M = \begin{pmatrix} M' & W_\varepsilon \end{pmatrix}$ has no type-4 NMF, thus concluding the proof of Proposition 3.3(4).

Remark 4.5. The existence of a suitable matrix W_ε can be understood in terms of upper semicontinuity of the nonnegative rank over the reals [4] and can be alternatively demonstrated using a nonconstructive argument that assumes only Claim 4.3 instead of the (stronger) Lemma 4.4; see Appendix B for details. We are not, however, aware of a simpler proof of Claim 4.3.

Proof of Lemma 4.4. The idea of the proof is to derive a contradiction from the assumption that there exists a stochastic matrix $\widetilde{W} \in \mathbb{R}_+^{6\times 5}$ that satisfies the constraints in Figure 6 and has an NMF $\widetilde{W} = L \cdot R$ of type 4, i.e., such that L matches the following zero pattern:

$$L = \begin{pmatrix} + & 0 & 0 & 0 & 0 \\ 0 & + & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

To this end, we use constraint propagation to successively derive lower and upper bounds for various entries of the matrices L and R until we reach a contradiction.

In our proof of the lemma, we use the following two assumptions, which are without loss of generality:

(A1) $L_{6,3} = \max\{L_{6,3}, L_{6,4}, L_{6,5}\}$, and

(A2) $L_{5,4} = \max\{L_{5,4}, L_{5,5}\}$.

Technically, these assumptions are used only in the proof of Claim 4.6 below.

We first demonstrate that Lemma 4.4 follows from the following two claims.

Claim 4.6. $L_{6,3} \geq 0.61$, $L_{5,4} \geq 0.9539$.

Claim 4.7. $L_{4,3} \geq 0.346$, $\max\{L_{3,3}, L_{3,4}\} \geq 0.0465$.

Proof of Lemma 4.4. Take the second inequality of Claim 4.7 and consider two cases:

- First, suppose that in Claim 4.7 it holds that $\max\{L_{3,3}, L_{3,4}\} = L_{3,3}$. Then $L_{3,3} \geq 0.0465$. Further, Claims 4.7 and 4.6 give lower bounds on $L_{4,3}$ and $L_{6,3}$, respectively. Since the elements of each column of L sum up to 1, it follows that $0.0465 + 0.346 + 0.61 \leq L_{3,3} + L_{4,3} + L_{6,3} \leq 1$. This is a contradiction.
- Otherwise, we have $\max\{L_{3,3}, L_{3,4}\} = L_{3,4} \geq 0.0465$. Recall that Claim 4.6 gives $L_{5,4} \geq 0.9539$. Hence $0.0465 + 0.9539 \leq L_{3,4} + L_{5,4} \leq 1$, which is also a contradiction. ∎

Our two goals now are to prove Claims 4.6 and 4.7. We achieve these using a sequence of auxiliary statements.

Claim 4.8. $0.29 \leq R_{2,4}$, $0.196 \leq R_{2,5}$.

Proof. Observe that all columns of $\widetilde{W}$ lie in the convex hull of columns of L since $\widetilde{W}_{:,j} = L \cdot R_{:,j}$. Consider the fourth and fifth columns $\widetilde{W}_{:,4}, \widetilde{W}_{:,5}$. Since $L_{:,2}$ is the only column of L with strictly positive second component, we have $\widetilde{W}_{2,4} = L_{2,2} \cdot R_{2,4}$ and $\widetilde{W}_{2,5} = L_{2,2} \cdot R_{2,5}$. Therefore,

$$0.29 \leq \widetilde{W}_{2,4} = L_{2,2} \cdot R_{2,4} \leq R_{2,4}, \qquad 0.196 \leq \widetilde{W}_{2,5} = L_{2,2} \cdot R_{2,5} \leq R_{2,5},$$

implying the claim. ∎

By omitting nonnegative terms from the equality $\widetilde{W}_{i,j} = L_{i,:} \cdot R_{:,j}$, we obtain the inequality $L_{i,k} \cdot R_{k,j} \leq \widetilde{W}_{i,j}$, which holds for all $1 \leq k \leq 5$. We can thus compute an upper bound on $L_{i,k}$ (resp., on $R_{k,j}$) if we know a lower bound on $R_{k,j}$ (resp., on $L_{i,k}$). We refer to this as computing *simple upper bounds* through $\widetilde{W}_{i,j}$.

Henceforth, we set $\varepsilon = 10^{-5}$, as in Figure 6.

Claim 4.9. *The matrix L satisfies the following constraints:*

$$\begin{array}{c|ccccc} & L_{:,1} & L_{:,2} & L_{:,3} & L_{:,4} & L_{:,5} \\ \hline L_{1,:} & & & & & \\ L_{2,:} & & 0.8 \leq \cdot & & & \\ L_{3,:} & & \cdot \leq 0.077 & & & \\ L_{4,:} & & \cdot \leq 0.12 & & & \\ L_{5,:} & & \cdot \leq 4\varepsilon & & & \\ L_{6,:} & & \cdot \leq 6\varepsilon & & & \end{array}.$$

Proof. First, note that, by Claim 4.8, $0.196 \leq R_{2,5}$. This lets us derive the following simple upper bounds through $\widetilde{W}_{3,5}, \widetilde{W}_{4,5}$, and $\widetilde{W}_{6,5}$:

$$L_{3,2} \leq \frac{0.015}{0.196} \leq 0.077, \qquad L_{4,2} \leq \frac{0.022}{0.196} \leq 0.12, \qquad L_{6,2} \leq \frac{\varepsilon}{0.196} \leq 6\varepsilon.$$

The remaining bounds are obtained as follows. The lower bound on $R_{2,4}$, taken from Claim 4.8, gives a simple upper bound $L_{5,2} \leq \varepsilon/0.29 \leq 4\varepsilon$ through $\widetilde{W}_{5,4}$. Now the upper bounds on $L_{i,2}$, where $3 \leq i \leq 6$, result in the inequality $L_{2,2} \geq 1 - (0.077 + 0.12 + 10\varepsilon) \geq 0.8$. ■

Now we are able to prove Claim 4.6.

Proof of Claim 4.6. We use the bounds of Claim 4.9 and the inequalities $\widetilde{W}_{2,1} \leq \varepsilon$, $\widetilde{W}_{6,1} \geq 0.62$, and $\widetilde{W}_{5,5} \geq 0.767$ from the statement of Lemma 4.4.

To begin with, the first column of $\widetilde{W}$ lies in the convex hull of $L_{:,2}$ and $L_{:,3}, L_{:,4}, L_{:,5}$. From the lower bound $L_{2,2} \geq 0.8$ we compute the simple upper bound $R_{2,1} \leq 2\varepsilon$ through $\widetilde{W}_{2,1}$. By our assumption (A1), $L_{:,3}$ has the largest sixth coordinate among $L_{:,3}, L_{:,4}$, and $L_{:,5}$, so from

$$0.62 \leq \widetilde{W}_{6,1} = L_{6,:} \cdot R_{:,1} \leq L_{6,2} \cdot R_{2,1} + (1 - R_{2,1}) \cdot L_{6,3} \leq L_{6,2} \cdot R_{2,1} + L_{6,3}$$

we obtain $L_{6,3} \geq 0.62 - 6\varepsilon \cdot 2\varepsilon \geq 0.61$, as claimed.

Furthermore, the fifth column of $\widetilde{W}$ also lies in the convex hull of $L_{:,2}$ and $L_{:,3}, L_{:,4}, L_{:,5}$. Recall that $L_{5,2}$ is at most 4ε, and $R_{2,5}$ is at least 0.196 by Claim 4.8. We then have

$$0.767 \leq \widetilde{W}_{5,5} = L_{5,:} \cdot R_{:,5} \leq L_{5,2} + (1 - R_{2,5}) \cdot \max\{L_{5,3}, L_{5,4}, L_{5,5}\},$$

yielding the bound $\max\{L_{5,3}, L_{5,4}, L_{5,5}\} \geq \frac{0.767-4\varepsilon}{1-0.196} \geq 0.9539$. As we already know that $L_{6,3} \geq 0.61$, we deduce that the maximum in the left-hand side cannot be attained by $L_{5,3}$, since the column vector $L_{:,3}$ is stochastic. Now, by our assumption (A2) we must have $L_{5,4} \geq 0.9539$. ■

Our next goal is prove Claim 4.7. Claim 4.10 and Claim 4.11, described below, take two consecutive steps in this direction.

Claim 4.10. $R_{5,2} \leq 50\varepsilon$, $R_{5,3} \leq 23\varepsilon$.

Proof. First, note that the matrix L satisfies the following constraints:

$$\begin{array}{c} \\ L_{1,:} \\ L_{2,:} \\ L_{3,:} \\ L_{4,:} \\ L_{5,:} \\ L_{6,:} \end{array} \begin{array}{c} \begin{array}{ccccc} L_{:,1} & L_{:,2} & L_{:,3} & L_{:,4} & L_{:,5} \end{array} \\ \begin{pmatrix} & & & & \\ & & & & \\ & \cdot \le 0.077 & & \cdot \le 0.0461 & \\ & \cdot \le 0.12 & & \cdot \le 0.0461 & \\ & & & 0.9539 \le \cdot & \\ & & 0.61 \le \cdot & & \end{pmatrix} \end{array} . \tag{14}$$

Indeed, the upper bounds on $L_{3,2}$ and $L_{4,2}$ are taken verbatim from Claim 4.9, and the lower bounds on $L_{6,3}$ and $L_{5,4}$ from Claim 4.6. The latter bound implies the upper bounds on $L_{3,4}$ and $L_{4,4}$.

We first prove the inequality $R_{5,2} \le 50\varepsilon$. By multiplying the row vector $\begin{pmatrix} 0 & 0 & 2 & 0 & 0 & -1 \end{pmatrix}$ with $\widetilde{W}_{:,4} = L \cdot R_{:,4}$, we obtain $2\widetilde{W}_{3,4} - \widetilde{W}_{6,4} = (2L_{3,:} - L_{6,:}) \cdot R_{:,4}$. Since the fourth column of $\widetilde{W}$ lies in the convex hull of $L_{:,2}$ and $L_{:,3}, L_{:,4}, L_{:,5}$, we also have

$$\begin{aligned} 2\widetilde{W}_{3,4} - \widetilde{W}_{6,4} &\le \max\{2L_{3,2} - L_{6,2},\ 2L_{3,3} - L_{6,3},\ 2L_{3,4} - L_{6,4},\ 2L_{3,5} - L_{6,5}\} \\ &\le \max\{2L_{3,2} - L_{6,2},\ 2L_{3,3} - L_{6,3},\ 2L_{3,4} - L_{6,4}\} + 2L_{3,5}. \end{aligned}$$

On the one hand, we have $2\widetilde{W}_{3,4} - \widetilde{W}_{6,4} \ge 0.21$, because $\widetilde{W}_{3,4} \ge 0.21$ and $\widetilde{W}_{6,4} \le 0.21$. On the other hand, $2L_{3,3} - L_{6,3} \le 2\,(1 - L_{6,3}) - L_{6,3} = 2 - 3L_{6,3}$. Hence

$$0.21 \le \max\{\underbrace{2L_{3,2}}_{\le 2\cdot 0.077}, \underbrace{2 - 3L_{6,3},}_{\le 2-3\cdot 0.61} \underbrace{2L_{3,4}}_{\le 2\cdot 0.0461}\} + 2L_{3,5}\,,$$

where the inequalities are taken from (14) and from the calculation above. Therefore, $L_{3,5} \ge 0.02$, from which we derive the simple upper bound $R_{5,2} \le 50\varepsilon$ through $\widetilde{W}_{3,2}$.

The second inequality, $R_{5,3} \le 23\varepsilon$, is proved in a similar way. By multiplying the row vector $\begin{pmatrix} 0 & 0 & 0 & 2 & 0 & -1 \end{pmatrix}$ with $\widetilde{W}_{:,4} = L \cdot R_{:,4}$, we obtain $2\widetilde{W}_{4,4} - \widetilde{W}_{6,4} = (2L_{4,:} - L_{6,:}) \cdot R_{:,4}$ and thus

$$2\widetilde{W}_{4,4} - \widetilde{W}_{6,4} \le \max\{2L_{4,2} - L_{6,2},\ 2L_{4,3} - L_{6,3},\ 2L_{4,4} - L_{6,4}\} + 2L_{4,5}.$$

On the one hand, we have $2\widetilde{W}_{4,4} - \widetilde{W}_{6,4} \ge 2 \cdot 0.27 - 0.21 \ge 0.33$. On the other hand, $2L_{4,3} - L_{6,3} \le 2(1 - L_{6,3}) - L_{6,3} = 2 - 3L_{6,3}$. Hence

$$0.33 \le \max\{\underbrace{2L_{4,2}}_{\le 2\cdot 0.12}, \underbrace{2 - 3L_{6,3},}_{\le 2-3\cdot 0.61} \underbrace{2L_{4,4}}_{\le 2\cdot 0.0461}\} + 2L_{4,5}\,,$$

where the inequalities are again taken from (14) and from the calculation above. It follows that $L_{4,5} \ge 0.045$, and we derive the simple upper bound $R_{5,3} \le \varepsilon/0.045 \le 23\varepsilon$ through $\widetilde{W}_{4,3}$. This completes the proof. ■

Claim 4.11. *The matrices L and R satisfy the following constraints:*

$$\begin{array}{c|ccccc} & L_{:,1} & L_{:,2} & L_{:,3} & L_{:,4} & L_{:,5} \\ \hline L_{1,:} & & & & & \\ L_{2,:} & & & & & \\ L_{3,:} & \cdot \leq 2\varepsilon & & & & \\ L_{4,:} & \cdot \leq 4\varepsilon & & & \cdot \leq 10\varepsilon & \\ L_{5,:} & & & & & \\ L_{6,:} & & & & & \end{array} \qquad \begin{array}{c|ccccc} & R_{:,1} & R_{:,2} & R_{:,3} & R_{:,4} & R_{:,5} \\ \hline R_{1,:} & & 0.8 \leq \cdot & 0.286 \leq \cdot & & \\ R_{2,:} & & & & & \\ R_{3,:} & & & & & \\ R_{4,:} & & & & & \\ R_{5,:} & & \cdot \leq 50\varepsilon & \cdot \leq 23\varepsilon & & \end{array}.$$

Proof. First, note that the constraints $R_{5,2} \leq 50\varepsilon$ and $R_{5,3} \leq 23\varepsilon$ are already known to us from Claim 4.10. We now show how to obtain the remaining five constraints.

Observe that the column $L_{:,1}$ is the only column of L that has a positive first component; hence it is the only column of L that contributes to the positive first component in the second and third columns of $\widetilde{W}$. Therefore, the following inequalities indeed hold:

$$0.286 \leq \widetilde{W}_{1,3} = L_{1,1} \cdot R_{1,3} \leq R_{1,3} \quad \text{and}$$
$$0.8 \leq \widetilde{W}_{1,2} = L_{1,1} \cdot R_{1,2} \leq R_{1,2}.$$

The latter inequality leads to the claimed simple upper bound $L_{3,1} \leq \varepsilon/0.8 \leq 2\varepsilon$ through $\widetilde{W}_{3,2}$. We further derive the following simple upper bounds:

- $R_{1,3} \leq 0.287/0.8 \leq 0.36$ through $\widetilde{W}_{1,3}$, since $L_{1,1} \geq L_{1,1} \cdot R_{1,2} = \widetilde{W}_{1,2} \geq 0.8$ by the above;
- $R_{3,3} \leq 0.32/0.61 \leq 0.53$ through $\widetilde{W}_{6,3}$, since $L_{6,3} \geq 0.61$ by Claim 4.6.

Since $\widetilde{W}_{:,3}$ lies in the convex hull of $L_{:,1}$ and $L_{:,3}, L_{:,4}, L_{:,5}$, we can deduce that $R_{4,3} = 1 - R_{1,3} - R_{3,3} - R_{5,3} \geq 1 - 0.36 - 0.53 - 23\varepsilon \geq 0.1$. Using this lower bound, $R_{4,3} \geq 0.1$, and the lower bound $R_{1,3} \geq 0.286$ obtained above, we deduce, through $\widetilde{W}_{4,3}$, simple upper bounds $L_{4,4} \leq 10\varepsilon$ and $L_{4,1} \leq 4\varepsilon$. This concludes the proof. ∎

We are now ready to prove Claim 4.7.

Proof of Claim 4.7. Here we will use only the result of Claim 4.11.

First, note that the second column of $\widetilde{W}$ lies in the convex hull of $L_{:,1}$, $L_{:,3}$, $L_{:,4}$, and $L_{:,5}$. We have

$$\begin{aligned} 0.07 \leq \widetilde{W}_{4,2} = L_{4,:} \cdot R_{:,2} &= L_{4,1}R_{1,2} + L_{4,3}R_{3,2} + L_{4,4}R_{4,2} + L_{4,5}R_{5,2} \\ &\leq \underbrace{L_{4,1}}_{\leq 4\varepsilon} + L_{4,3}\underbrace{(1 - R_{1,2})}_{\leq 0.2} + \underbrace{L_{4,4}}_{\leq 10\varepsilon} + \underbrace{R_{5,2}}_{\leq 50\varepsilon}, \end{aligned}$$

which gives us the lower bound $0.346 \leq L_{4,3}$.

Similarly, consider the third column of $\widetilde{W}$ and observe that

$$\begin{aligned} 0.0335 \leq \widetilde{W}_{3,3} = L_{3,:} \cdot R_{:,3} &= L_{3,1}R_{1,3} + L_{3,3}R_{3,3} + L_{3,4}R_{4,3} + L_{3,5}R_{5,3} \\ &\leq \underbrace{L_{3,1}}_{\leq 2\varepsilon} + \max\{L_{3,3}, L_{3,4}\}\underbrace{(1 - R_{1,3})}_{\leq 0.714} + \underbrace{R_{5,3}}_{\leq 23\varepsilon}. \end{aligned}$$

The lower bound $\max\{L_{3,3}, L_{3,4}\} \geq 0.0465$ follows. ∎

As we have seen above, Lemma 4.4 follows from Claims 4.6 and 4.7.

5. Conclusions.

In this paper we have solved the Cohen–Rothblum problem, showing that nonnegative ranks over $\mathbb{R}$ and over $\mathbb{Q}$ may differ. More precisely, our construction applies to matrices of rank 4 and higher. It was already known to Cohen and Rothblum [9] that nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ coincide for matrices of rank at most 2, and Kubjas, Robevas, and Sturmfels [16] showed that this also holds for matrices of nonnegative rank (over $\mathbb{R}$) at most 3. The remaining open question is whether nonnegative ranks over $\mathbb{R}$ and over $\mathbb{Q}$ differ for rank-3 matrices whose nonnegative rank (over $\mathbb{R}$) is at least 4—or whether our example is optimal in this sense.

As our results show that the nonnegative ranks over $\mathbb{R}$ and $\mathbb{Q}$ are different functions, the computability question emerges. It has long been known (see, e.g., Cohen and Rothblum [9]) that the nonnegative rank over $\mathbb{R}$ is computable, via a reduction to the existential theory of the reals, which in turn can be decided in PSPACE. (Recently, Shitov proposed a reduction in the converse direction, i.e., from the existential theory of the reals to NMF [24].) In contrast, it is not known whether the nonnegative rank over $\mathbb{Q}$ is computable. While there is a natural reduction to the decision problem for the existential theory of the rationals, the decidability of the latter is a long-standing and very prominent open question [21].

Finally, we would like to point out that the complexity of the following geometric problem closely linked to NMF, the *nested polytope* problem, is not fully known. This problem asks, given an ordered field $\mathbb{F}$ and polytopes $\mathcal{S} \subseteq \mathcal{T}$ in $\mathbb{F}^n$, whether there exists a *simple* polytope $\mathcal{N}$ such that $\mathcal{S} \subseteq \mathcal{N} \subseteq \mathcal{T}$ (cf. Gillis and Glineur [14]). The definition of "simple" can be either "having at most k vertices," or "having at most k facets," or a combination of both. For $\mathbb{F} = \mathbb{R}$, minimizing the number of vertices or, dually, facets is known to require irrational numbers [7] even in the case of full-dimensional $\mathcal{S}$. While for some representations of the polytopes such questions are known to be NP-hard (see, e.g., Das and Goodrich [10]), their precise complexity is not known in general.

Appendix A. Uniqueness of type-1 NMFs of M.

In this appendix, we strengthen Proposition 3.3(1) to show that any type-1 NMF of M coincides with the one given in equation (2), up to a permutation of the columns of W and the rows of $\begin{pmatrix} H' & H_\varepsilon \end{pmatrix}$. Together with the other parts of Proposition 3.3, this implies that the NMF (2) is the only 5-dimensional stochastic NMF of the matrix M, up to permutations.

Proposition A.1. *If $M = L \cdot R$ is a type-1 NMF, then L is equal to W up to a permutation of its columns.*

Proof. We recall from Figure 3 that the supporting polygon $\mathcal{S}_{q_1^*}$, nested between the triangle $\triangle r_1 r_2 r_3$ and the polygon $\mathcal{P}_0$, is the triangle $\triangle q_1^* q_3^* q_2^*$. Similarly, as seen in Figure 4, the supporting polygon $\mathcal{S}_{q_1^*}$, nested between the triangle $\triangle r_4 r_5 r_6$ and the polygon $\mathcal{P}_1$, is the triangle $\triangle q_1^* q_5^* q_4^*$. We have already shown that $q_1 = q_1^*$. In the following, we show that $q_i = q_i^*$ for each $i \in \{2, 3, 4, 5\}$.

Towards a contradiction, suppose that $q_2 \neq q_2^*$ or $q_3 \neq q_3^*$. Let us consider the case when $q_2 \neq q_2^*$. Observe that triangles $\triangle q_1^* q_3^* q_2^*$ and $\triangle q_1^* q_3 q_2$ are both nested between $\triangle r_1 r_2 r_3$ and $\mathcal{P}_0$. The fact that $\triangle r_1 r_2 r_3 \subseteq \triangle q_1^* q_3 q_2$ implies that vertices q_3 and q_2 lie to the right of (or on) directed line segments $q_1^* q_3^*$ and $q_2^* q_1^*$, respectively. Since, moreover, $q_3, q_2 \in \mathcal{P}_0$, it holds that vertex q_3 lies to the left of (or on) directed line segment $q_3^* q_2^*$, whereas vertex q_2 lies strictly to the left of $q_3^* q_2^*$. However, this implies that the point r_2 is to the right of directed line segment $q_3 q_2$, which contradicts the assumption that $\triangle r_1 r_2 r_3 \subseteq \triangle q_1^* q_3 q_2$. The case $q_3 \neq q_3^*$ analogously leads to a contradiction. We conclude that $q_2 = q_2^*$ and $q_3 = q_3^*$. Analogously, using Lemma 4.2 one can show that $q_4 = q_4^*$ and $q_5 = q_5^*$.

Since $f(q_i) = L_{:,i}$ and $f(q_i^*) = W_{:,i}$ for each $i \in \{2, 3, 4, 5\}$, we conclude that $\{L_{:,2}, L_{:,3}\} = \{W_{:,2}, W_{:,3}\}$ and $\{L_{:,4}, L_{:,5}\} = \{W_{:,4}, W_{:,5}\}$. Therefore, the NMF $M = L \cdot R$ coincides with the one given in (2), up to a permutation of the columns of W and the rows of $\begin{pmatrix} H' & H_\varepsilon \end{pmatrix}$. ■

Appendix B. A nonconstructive approach to defining W_ε. Instead of deducing the result of section 4.5 from Lemma 4.4, one can alternatively rely on its weaker form, Claim 4.3, and give a nonconstructive proof of the existence of an appropriate W_ε (satisfying the three desiderata given as bullet points in section 4.5 on page 298) via a topological argument that we sketch below. However, we emphasize that we do not know how to prove Claim 4.3 without following the arguments that prove Lemma 4.4.

Proposition B.1. *There exists a 6×5 matrix such that*
- *its entries are rational,*
- *its columns belong to the convex hull of the columns of W, and*
- *it has no type-4 NMF.*

Proof. We first employ the geometric constructions of section 4.1 to argue that every neighborhood of the matrix W contains a rational matrix that factors through W, i.e., whose columns belong to the convex hull of the columns of W. Indeed, consider the set $\mathcal{F}$ of all stochastic real matrices of size 6×5 that have a stochastic NMF with left factor W. Observe that $\mathcal{F}$ can be characterized as the set of matrices whose columns lie in the image under f of a full-dimensional set in $\mathbb{R}^3$, namely of the convex hull of $q_1^*, \ldots, q_5^*$. Since the map f is specified by matrices C and d with rational coefficients, it immediately follows that the set of rational matrices is dense in $\mathcal{F}$. As every δ-neighborhood of the matrix W includes some 3-dimensional subset of $\mathcal{F}$, it also contains a rational matrix W_δ from $\mathcal{F}$, as we wished to prove.

Now assume for the sake of contradiction that every rational matrix in the set $\mathcal{F}$ has a type-4 NMF. Then the matrices W_δ from above also have type-4 NMFs $W_\delta = L_\delta \cdot R_\delta$ for all $\delta > 0$. By compactness, there exists a subsequence of matrices W_δ with decreasing δ such that the corresponding sequences L_δ and R_δ converge. Taking the limit, we arrive at the equality $W = L \cdot R$, where the right-hand side is also a type-4 NMF—which contradicts Claim 4.3. This completes the proof. (Note that Lemma 4.4 contains a constructive version of this argument.) ■

It is worth mentioning that this reasoning follows similar lines as the *upper semicontinuity* argument for nonnegative rank [4]: the nonnegative rank of any (rational or irrational) matrix W_ε which is entrywise close enough to W can only be greater than or equal to that of W.

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