On the complexity of nonnegative matrix factorization

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Abstract

Nonnegative matrix factorization (NMF) has become a prominent technique for the analysis of image databases, text databases and other information retrieval and clustering applications. In this report, we define an exact version of NMF. Then we establish several results about exact NMF: (1) that it is equivalent to a problem in polyhedral combinatorics; (2) that it is NP-hard; and (3) that a polynomial-time local search heuristic exists.

1 Nonnegative matrix factorization

Nonnegative matrix factorization (NMF) has emerged in the past decade as a powerful tool for clustering data and finding features in datasets. Lee and Seung [12] showed that NMF can find features in image databases, and Hofmann [10] showed that probabilistic latent semantic analysis, a variant of NMF, can effectively cluster documents according to their topics. Cohen and Rothblum [5] describe applications for NMF in probability, quantum mechanics and other fields.

Nonnegative matrix factorization is defined as the following problem. The input is (A, k), where A is an $m \times n$ matrix with nonnegative entries, and k is an integer such that $1 \le k \le \min(m, n)$. The output is a pair of matrices (W, H) with $W \in \mathbf{R}^{m \times k}$ and $H \in \mathbf{R}^{k \times n}$ such that W and W both have nonnegative entries and such that $W \in \mathbf{R}^{m \times k}$. The precise sense in which WH approximates W may vary from one author to the next. Furthermore, some authors seek sparsity in either W or W or W or W both. Sparsity may be imposed as a term in the objective function [11].

The algorithms proposed by [10, 11, 12] and others for NMF have generally been based on local improvement heuristics. Another class of heuristics is based on greedy rank-one downdating [1, 2, 3, 8]. No algorithm proposed in the literature comes with a guarantee of optimality. This suggests that solving NMF to optimality may be a difficult problem, although to the best of our knowledge this has never been established formally.

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The main purpose of this paper is to provide the proof that NMF is NP-hard. This paper considers a particular version of NMF that we call *exact NMF*, which is defined as follows.

EXACT NMF: The input is a matrix $A \in \mathbf{R}^{m \times n}$ with nonnegative entries whose rank is exactly $k, k \geq 1$. The output is a pair of matrices (W, H), where $W \in \mathbf{R}^{m \times k}$ and $H \in \mathbf{R}^{k \times n}$, W and H both have nonnegative entries, and A = WH. If no such (W, H) exist, then the output is a statement of nonexistence of a solution. The decision version of EXACT NMF takes the same input and gives as output **yes** if such a W and H exists else it outputs **no**.

Implicit in the statement of exact NMF is an assumption that the rank of A is known. If A is specified as rational data, then its rank may determined in polynomial time via reduction to row-echelon form [6]. In practice, one would usually prefer singular value decomposition to determine rank(A) [9].

Observe that for any reasonable definition of the approximation version of NMF (that is, the version described earlier in which $\operatorname{rank}(A)$ is not constrained and in which one requires $A \approx WH$ instead of exact equality), an optimal algorithm when presented with an A whose rank is exactly k ought to solve the exact NMF problem. Thus, the "standard" NMF problem using any norm is a generalization of EXACT NMF. Therefore, any hardness result that applies to exact NMF (such as our hardness result) would presumably apply to most approximation versions as well.

A different generalization of EXACT NMF is the problem of nonnegative rank determination due to Cohen and Rothblum, which asks, given $A \in \mathbf{R}^{m \times n}$ with nonnegative entries, find the minimum value of k such that A = WH, $W \in \mathbf{R}^{m \times k}$, $H \in \mathbf{R}^{k \times n}$, and W, H have nonnegative entries. Cohen and Rothblum give a super-exponential time algorithm for this problem. Since nonnegative rank determination is a generalization of EXACT NMF, our result shows that it is also NP-hard.

The proof of NP-hardness of EXACT NMF has two parts: In Section 2 we show equivalence between EXACT NMF and a problem in polyhedral combinatorics that we call INTERMEDIATE SIMPLEX, and in Section 3 we show the NP-hardness of this problem. A side result emerging from the proof of equivalence of EXACT NMF to INTERMEDIATE SIMPLEX is that certain local-search heuristic for EXACT NMF can be solved with linear programming (Section 4).

2 Equivalence to Intermediate Simplex

In this section, we show an equivalence between the EXACT NMF and a problem in polyhedral combinatorics that we call INTERMEDIATE SIMPLEX. Although the focus in this section is on the decision version of these problems, it is apparent from the proofs that the search-versions could also be reduced to each other. The reductions use a number of arithmetic operations polynomial in m and n and are therefore polynomial-time for both the usual Turing machine model and the real-number model of Blum et al. [4].

A problem related to INTERMEDIATE SIMPLEX was proposed by Cohen and Rothblum [5] and show to be equivalent to nonnegative rank determination. Therefore, their results to some extent imply the results of this section. Nonetheless, we present the equivalence here in order to provide detail for our claim that all reductions are polynomial time.

The equivalence is shown in three steps by first showing an equivalence to a problem denoted P1.

<u>**P1**</u>: Given matrices $W_0 \in \mathbf{R}^{m \times k}$ and $H_0 \in \mathbf{R}^{k \times n}$ such that each has rank k and such that all entries of W_0H_0 are nonnegative, does there exist a nonsingular matrix $Q \in \mathbf{R}^{k \times k}$ such that W_0Q^{-1} and QH_0 both have all nonnegative entries?

Theorem 1. There is a polynomial-time reduction from EXACT NMF to P1 and vice versa.

Proof. First we demonstrate the reduction of EXACT NMF to P1. Suppose that we have an NMF instance, that is, a nonnegative matrix A of rank exactly k. In polynomial time (using, e.g., reduction to row-echelon form) one can factor $A = W_0H_0$ such that $W_0 \in \mathbf{R}^{m \times k}$ and $H_0 \in \mathbf{R}^{k \times n}$. (This factorization does not solve exact NMF since the signs of the entries of W_0 and H_0 are unknown.) We claim that the original instance of EXACT NMF is a yes-instance iff the instance of P1 is a yes-instance. For one direction, suppose the instance of EXACT NMF is a ves-instance, and suppose W, H are solutions to exact NMF. Then clearly Range(A) = Range(W) = Range(W₀), which is a dimension-k subspace of \mathbf{R}^n , and similarly Range (A^T) = Range (H^T) = Range (H_0^T) . This means that there exist two nonsingular $k \times k$ nonsingular matrices, say P, Q, such that $W = W_0 P$ and $H = QH_0$. Thus, the equation $WH = W_0H_0$ may be rewritten as $W_0PQH_0 = W_0H_0$. Notice that W_0 has a left inverse and H_0 has a right-inverse since W_0 has full column rank and H_0 has full row rank. Thus, the previous equation simplifies to PQ = I (where I denotes the $k \times k$ identity matrix), i.e., $P = Q^{-1}$. Thus, W_0Q^{-1} and QH_0 both have nonnegative entries, so the instance of P1 is a yes-instance. Conversely, suppose the instance of P1 is a yes-instance. Then there exists Q such that $W = W_0 Q^{-1}$ and $H = QH_0$ both have all nonnegative entries, and $WH = W_0H_0 = A$, so the instance of exact NMF is a yes-instance.

For the opposite reduction, suppose we start with an instance (W_0, H_0) of P1. Let $A = W_0H_0$; then A is nonnegative and has rank k. We claim that the instance of A is a yes-instance if and only if the instance of P1 is a yes-instance. The proof uses essentially the same arguments as in the previous paragraph.

In order to simplify the main proof in this section, it is helpful to define a slightly restricted version of P1 as follows by requiring the last column of W_0 to be all 1's:

RESTRICTED P1: Given matrices $W_0 \in \mathbf{R}^{m \times k}$ and $H_0 \in \mathbf{R}^{k \times n}$ such that (1) each has rank k; (2) all entries of W_0H_0 are nonnegative; and (3) the last column of W_0 is all 1's, does there exists a nonsingular matrix $Q \in \mathbf{R}^{k \times k}$ such that W_0Q^{-1} and QH_0 both have all nonnegative entries?

Theorem 2. There is a polynomial-time reduction from P1 to RESTRICTED P1 and vice versa.

Proof. Given an instance (W_0, H_0) of P1, we can produce an instance of RESTRICTED P1 as follows. First, delete all rows of W_0 that are identically 0's. This does not affect the

rank of W_0 , nor does it affect whether the product W_0H_0 is nonnegative. Finally, if Q is a solution problem P1 prior to deletion of identically zero rows, then it is still a solution afterwards and vice versa.

For the next step, let \hat{Q} be a $k \times k$ nonsingular matrix chosen such that $\hat{Q}H_0\mathbf{e} = \mathbf{e}_k$. Here, $\mathbf{e} \in \mathbf{R}^n$ denotes the vector of all 1's, and $\mathbf{e}_k \in \mathbf{R}^k$ denotes the last column of the $k \times k$ identity matrix. Such a \hat{Q} is guaranteed to exist because $H_0\mathbf{e}$ cannot be zero: $W_0H_0\mathbf{e}$ is the sum of columns of W_0H_0 , which cannot be zero since the columns of W_0H_0 are all nonnegative and W_0H_0 is not identically zero by the assumption of rank at least 1. Then observe that $(W_0\hat{Q}^{-1}, \hat{Q}H_0)$ is a yes-instance of P1 iff (W_0, H_0) is a yes-instance. Such a \hat{Q} may be found in polynomial time; for example, any $k \times k$ nonsingular matrix whose last column is $H_0\mathbf{e}$ may be taken as \hat{Q}^{-1} , and matrix inversion is polynomial-time in the Turing machine model [6].

Next, we observe that the last column of $W_0\hat{Q}^{-1}$ is $W_0\hat{Q}^{-1}\mathbf{e}_k = W_0\hat{Q}^{-1}\hat{Q}H_0\mathbf{e} = W_0H_0\mathbf{e}$. We already argued above that this vector is nonzero, but now we will argue more strongly that every entry of $W_0H_0\mathbf{e}$ is positive. First, note that $W_0H_0\mathbf{e}$ is the sum of columns of the nonnegative matrix W_0H_0 , and hence all its entries are at least nonnegative. Focus on entry i of $W_0H_0\mathbf{e}$; since it is a sum of nonnegative terms, then if it were zero then the entire ith row of W_0H_0 would have to be zeros. This means that the ith row of W_0 is orthogonal to every column of H_0 . But since H_0 has full rank, this is possible only if the ith row of W_0 is identically 0. However, this possibility is ruled out since we deleted identically zero rows of W_0 .

Thus, the last column of $W_0\hat{Q}^{-1}$ contains all positive entries. Therefore, we can consider the instance of P1 given by $(DW_0\hat{Q}^{-1},\hat{Q}H_0)$ where D is an $m\times m$ positive definite diagonal matrix with diagonal entries chosen to make the last column of $DW_0\hat{Q}^{-1}$ equal to 1. This instance of P1 is a yes-instance only if the original instance was a yes-instance, because multiplying the first factor by a positive definite diagonal matrix does not affect the signs of W_0H_0 nor of $W_0\hat{Q}^{-1}Q^{-1}$.

The opposite reduction, namely the one from from RESTRICTED P1 to P1, is trivial since any instance of RESTRICTED P1 is also an instance of P1.

Now finally we get to the main new problem of this section.

INTERMEDIATE SIMPLEX: We are given a polyhedron $P = \{\mathbf{x} \in \mathbf{R}^{k-1} : A\mathbf{x} \ge \mathbf{b}\}$ where $A \in \mathbf{R}^{n \times (k-1)}$ and $\mathbf{b} \in \mathbf{R}^n$ such that $[A, \mathbf{b}]$ has rank k. We are also given a set $S \subset \mathbf{R}^{k-1}$ of m points that are all contained in P and that are not all contained in any hyperplane (i.e., they affinely span \mathbf{R}^{k-1}). The question is whether there exists a (k-1)-simplex T such that $S \subset T \subset P$.

Theorem 3. There is a polynomial-time reduction from RESTRICTED P1 to INTER-MEDIATE SIMPLEX and vice versa.

Proof. We will prove that both reductions exist at the same time by exhibiting a bijection between instances of RESTRICTED P1 and instances of INTERMEDIATE SIMPLEX such that both directions of the bijection can be computed in polynomial time.

Given an instance (W_0, H_0) of RESTRICTED P1, we produce an instance of INTER-MEDIATE SIMPLEX as follows. The polytope $P \subset \mathbf{R}^{k-1}$ is given by $\{\mathbf{x} \in \mathbf{R}^{k-1} : H_0(1 : \mathbf{x}) = H_0(1 : \mathbf{x}) : H_0(1 : \mathbf{x}) :$

k-1,: $)^T\mathbf{x} \geq -H_0(k,:)^T$. (This constraint may be written more compactly as $H_0^T[\mathbf{x};1] \geq \mathbf{0}$.) The set S of m points in P is given by $S = \{W_0(1,1:k-1)^T,\ldots,W_0(m,1:k-1)^T\}$. The inverse mapping of this transformation starts with an instance of INTERMEDIATE SIMPLEX given by $P = \{\mathbf{x}: A\mathbf{x} \geq \mathbf{b}\}, A \in \mathbf{R}^{m \times (k-1)} \text{ and } S = \{\mathbf{x}_1,\ldots,\mathbf{x}_m\} \text{ and produces an instance of RESTRICTED P1 given by}$

$$W_0 = \begin{pmatrix} \mathbf{x}_1^T & 1\\ \vdots & \vdots\\ \mathbf{x}_m^T & 1 \end{pmatrix}$$

and $H_0 = [A^T; -\mathbf{b}^T].$

We first show that all side-constraints present in the statement of RESTRICTED P1 and INTERMEDIATE SIMPLEX are satisfied. The side-constraint that $[A, \mathbf{b}]$ has rank k is equivalent (under this bijection) to the side-constraint that H_0 has rank k. The side-constraint that $\mathbf{x}_1, \ldots, \mathbf{x}_m$ affinely span \mathbf{R}^{k-1} is equivalent to requiring that $[\mathbf{x}_1; 1], \ldots, [\mathbf{x}_m; 1]$ linearly span \mathbf{R}^k , i.e., to the side-constraint that W_0 has rank k. Finally, the side constraint that $S \subset P$ means that $A\mathbf{x}_i \geq \mathbf{b}$ for $i = 1, \ldots, m$, i.e., $[A, -\mathbf{b}][\mathbf{x}_i; 1] \geq 0$, which is hence equivalent to the side-constraint that all entries of W_0H_0 are nonnegative.

We now show that the above bijection in both directions maps yes-instances to yes-instances. Let (S, P) be an instance of INTERMEDIATE SIMPLEX and (W_0, H_0) the corresponding instance of RESTRICTED P1. Let T be a putative solution to the instance of INTERMEDIATE SIMPLEX. Let its vertices be $\mathbf{g}_1, \ldots, \mathbf{g}_k$, which are vectors in \mathbf{R}^{k-1} . The condition that $T \subset P$ is equivalent to requiring $\mathbf{g}_1, \ldots, \mathbf{g}_k \in P$, i.e., to $H_0^T[\mathbf{g}_i; 1] \geq \mathbf{0}$ for each $i = 1, \ldots, k$. If we let

$$G = \begin{pmatrix} \mathbf{g}_1 & \cdots & \mathbf{g}_k \\ 1 & \cdots & 1 \end{pmatrix}, \tag{1}$$

then we have shown that the condition $T \subset P$ is equivalent to requiring $H_0^T G$ has all nonnegative entries.

The condition that $S \subset T$ means that for all i = 1, ..., m, $\mathbf{x}_i \in T$. Recall that, by definition, a vector is inside a simplex if it is a convex combination of its vertices. Let \mathbf{q}_i be the putative vector of coefficients of the convex combination that expresses \mathbf{x}_i in the hull of the vertices of T, for i = 1, ..., m. In other words,

$$[\mathbf{g}_1, \dots, \mathbf{g}_k] \mathbf{q}_i = \mathbf{x}_i, \tag{2}$$

plus the requirements that the entries of \mathbf{q}_i are nonnegative and sum to 1. The latter constraint may be combined with (2) to write $G\mathbf{q}_i = [\mathbf{x}_i; 1]$ where G is as in (1), i.e., $\mathbf{q}_i = G^{-1}W_0(i,:)^T$. The hypothesis that $S \subset T$ is thus equivalent to the condition that each entry of $G^{-1}W_0^T$ for each $i = 1, \ldots, m$ is nonnegative, i.e., all entries of $G^{-1}W_0^T$ must be nonnegative. Hence, we have shown that T is a solution to the instance (S, P) if and only if G^T is a solution to the instance (W_0, H_0) of RESTRICTED P1.

The argument is essentially the same in the other direction. Given an instance (W_0, H_0) of RESTRICTED P1, let (S, P) be the corresponding instance of INTERMEDIATE SIMPLEX. Let Q be a putative solution to the RESTRICTED P1 instance, and let $\mathbf{g}_1, \ldots, \mathbf{g}_k$

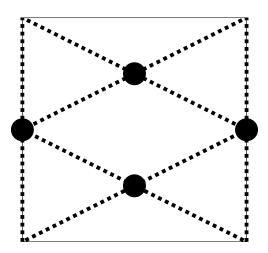


Figure 1: Illustration of Lemma 1. The four large dots are the points in S; the thin solid line is the boundary of P, and the two triangles indicated with thick dashed lines are the two possible solutions T_0 and T_1 .

be the columns of Q^T . Using the arguments in the previous paragraph shows that W_0Q^{-1} and QH_0 have nonnegative entries iff $S \subset T$ and $T \subset P$.

An easy consequence of our transformation of EXACT NMF to INTERMEDIATE SIMPLEX is the observation that when $\operatorname{rank}(A) = 2$, the NMF instance is always a yes-instance. The reason is that the resulting instance of INTERMEDIATE SIMPLEX is 1-dimensional in which case P is an interval. However, if P is an interval then it is already a simplex, so one could take T = P to solve the instance. This observation yields a simple linear-time algorithm to find an exact nonnegative factorization of A case $\operatorname{rank}(A) = 2$. case. This result was first established by Cohen and Rothblum [5], who also propose a simple linear-time algorithm.

3 INTERMEDIATE SIMPLEX is NP-hard

In this section, we will argue that the problem INTERMEDIATE SIMPLEX introduced in the previous section is NP-hard.

Before delving into the statement of the main theorem and its proof, we first state the following simpler lemma and proof. This lemma describes the 'gadget' used in the main theorem below to encode a setting of a boolean variable.

Lemma 1. Consider the following instance of INTERMEDIATE SIMPLEX: the polyhedron P is given by $P = \{(x,y) \in \mathbf{R}^2 : 0 \le x,y \le 1\}$, while the set S is given by $\{(0,1/2),(1,1/2),(1/2,1/4),(1/2,3/4)\}$. This instance has precisely two solutions T_0 or T_1 defined by $T_0 = \text{hull}\{(0,0),(0,1),(1,1/2)\}$ and $T_1 = \text{hull}\{(1,0),(1,1),(0,1/2)\}$.

A diagram of the lemma is given in Fig. 1. It is easy to check that the side-constraints of INTERMEDIATE SIMPLEX (that $S \subset P$, that $[A, \mathbf{b}]$ has full column rank, that S affinely spans \mathbb{R}^2) are satisfied by the above instance.

Proof. The fact that $S \subset T_i \subset P$, i = 0, 1, is elementary to check. The fact that there are no other solutions is proved as follows. Suppose T is a solution. Let E_0 and E_1 be the two parallel edges of P given by $E_0 = \{0\} \times [0,1]$ and $E_1 = \{1\} \times [0,1]$. Observe that the point $(0,1/2) \in S$ lies on E_0 , which means that the face of T containing (0,1/2) must be either 0 or 1-dimensional, and if it is 1-dimensional then it must be a subset of E_0 . Similarly, (1, 1/2) must lie on a 0- or 1-dimensional boundary of T. It is not possible for both (0,1/2) and (1,1/2) to lie on 1-dimensional boundaries since a triangle cannot have two parallel edges. It is also not possible for both (0,1/2) and (1,1/2) to be 0-dimensional boundaries because in this case $[0,1] \times \{1/2\}$ would be a bounding segment of T. Then all of T would have to be either above or below the segment, but then T would fail to cover either (1/2, 1/4) or (1/2, 3/4), points in S. Thus, the only possibilities are (1) that (0,1/2) is a vertex of T, and T has an edge that is a subset of E_1 , or (2) that (1,1/2) is a vertex of T, and T has an edge that is a subset of E_0 . But now one checks that in either case, in order to cover the two points (1/2, 3/4) and (1/2, 1/4), the entire edge E_0 or E_1 must be taken as an edge of T.

We now turn to the main result for this section, namely, the NP-hardness of INTER-MEDIATE SIMPLEX. In particular, we reduce 3-SAT [7] to this problem. Our reduction uses integers whose magnitude is polynomial in the instance of the 3-SAT instance, and hence our result is 'strong' NP-hardness. Recall that an instance of 3-SAT involves p boolean variables denoted x_1, \ldots, x_p and q clauses denoted c_1, \ldots, c_q . Each clause is a disjunction of three literals, where a literal is either a variable x_j or its complement \tilde{x}_j . An instance of 3-SAT is a yes-instance if and only if there exists a setting of the variables, that is, an assignment of a value of either 0 or 1 to each variable, such that each clause is satisfied, i.e., at least one of its three literals is 1. It is assumed that the same variable does not occur twice (either in complemented or plain form) in any particular clause.

Given such an instance of 3-SAT, we define the following instance of INTERMEDIATE SIMPLEX. It contains 3p + q variables (i.e., k - 1 = 3p + q) denoted $s_i, t_i, u_i, i = 1, ..., p$, and $v_j, j = 1, ..., q$. These variables are written as $(\mathbf{s}, \mathbf{t}, \mathbf{u}, \mathbf{v})$ for short. The polyhedron P is defined by the following inequalities:

$$P = \left\{ \begin{array}{ll} (\mathbf{s}, \mathbf{t}, \mathbf{u}, \mathbf{v}) : & \mathbf{0} \leq \mathbf{s} \leq \mathbf{u}, \\ & \mathbf{0} \leq \mathbf{t} \leq \mathbf{u}, \\ & \mathbf{0} \leq \mathbf{u} \leq \mathbf{e}, \\ & \mathbf{v} \geq \mathbf{0}, \\ & s_i - 2t_i \leq v_j \quad \text{whenever } \tilde{x}_i \in c_j, \\ & 2t_i - 2s_i - u_i \leq v_j \quad \text{whenever } x_i \in c_j \end{array} \right\}.$$

$$(3)$$

Here, **e** denotes the vector of all 1's. In the above usage, $\mathbf{e} \in \mathbf{R}^p$, but we shall also use **e** to denote the vector of all 1's in \mathbf{R}^q .

Let \mathbf{e}_i denote the *i*th column of the identity matrix (either the $p \times p$ or $q \times q$ identity). The set of points S is defined as follows. Each of the points in the following equation is

also given a name for future reference.

$$S = \begin{cases} \mathbf{0}, & (\mathbf{e}/(4p), \mathbf{e}/(4p), \mathbf{e}/(2p), 2.5\mathbf{e}/(8p)) & (\equiv \mathbf{b}), \\ (\mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{e}_j) & (\equiv \mathbf{h}_j), & j = 1, \dots, q \\ (\mathbf{0}, \mathbf{e}_i/4, \mathbf{e}_i/2, \mathbf{e}) & (\equiv \mathbf{r}_i^1), & i = 1, \dots, p \\ (\mathbf{e}_i/2, \mathbf{e}_i/4, \mathbf{e}_i/2, \mathbf{e}) & (\equiv \mathbf{r}_i^2), & i = 1, \dots, p \\ (\mathbf{e}_i/4, \mathbf{e}_i/8, \mathbf{e}_i/2, \mathbf{e}) & (\equiv \mathbf{r}_i^3), & i = 1, \dots, p, \\ (\mathbf{e}_i/4, 3\mathbf{e}_i/8, \mathbf{e}_i/2, \mathbf{e}) & (\equiv \mathbf{r}_i^4), & i = 1, \dots, p \end{cases}$$

$$(4)$$

Let us first confirm that the side-constraints of INTERMEDIATE SIMPLEX are satisfied by this instance. Since $\mathbf{0} \in S$, S affinely spans \mathbf{R}^{3p+q} iff it linearly spans \mathbf{R}^{3p+q} . Points \mathbf{h}_j , $j=1,\ldots,q$, span the subspace defined by the last q coordinate entries. Fix some $i \in \{1,\ldots,p\}$. Subtract $\mathbf{h}_1 + \ldots + \mathbf{h}_q$ from the three points $\mathbf{r}_i^1, \mathbf{r}_i^2, \mathbf{r}_i^3$. This yields three points whose nonzero entries are restricted to the (s_i,t_i,u_i) positions; in these positions the three points have coordinate entries (0,1/4,1/2), (1/2,1/4,1/2) and (1/4,1/8,1/2), which are linearly independent. Thus, the subspace indexed by (s_i,t_i,u_i) is spanned by S. This is true for all i, so therefore the points in S span all of \mathbf{R}^{3p+q} .

The next side-constraint is that the linear inequalities defining P are independent. One checks that the constraints $\mathbf{s} \geq \mathbf{0}$, $\mathbf{t} \geq \mathbf{0}$, $\mathbf{u} \geq \mathbf{0}$, $\mathbf{v} \geq \mathbf{0}$ imply that the constraint matrix contains a $(3p+q) \times (3p+q)$ identity matrix and hence has independent columns. We can also check that the right-hand side is independent of the columns of the matrix; if it were dependent, then there would be a point such that all the constraints are active at that point, which is obviously impossible (e.g., the constraints $\mathbf{u} \geq \mathbf{0}$ and $\mathbf{u} \leq \mathbf{e}$ cannot be simultaneously active). The final side-constraint is that $S \subset P$, which is an elementary matter to check.

The main theorem of this section is as follows.

Theorem 4. The instance of 3-SAT is a yes-instance if and only if the above instance of INTERMEDIATE SIMPLEX is a yes-instance. In other words, the 3-SAT instance has a satisfying assignment if and only if there exists a simplex T such that $S \subset T \subset P$.

Proof. First, let us choose some terminology for the coordinates of \mathbf{R}^{3p+q} . The individual coordinates may be denoted by s_i , t_i , u_i or v_j for $i=1,\ldots,p$ and $j=1,\ldots,q$. Collectively, the three coordinates (s_i,t_i,u_i) are called the " x_i coordinates" since they correspond to the *i*th boolean variable in the 3-SAT instance.

Let T be a solution to the instance of INTERMEDIATE SIMPLEX. From T we will construct a satisfying assignment σ for the 3-SAT instance. Clearly T has exactly 3p+q+1 vertices. Observe first that the point $\mathbf{0}$ is an extreme point of P and also lies in S, and therefore one vertex of T must be $\mathbf{0}$.

Similarly, observe that each \mathbf{h}_j , j = 1, ..., q, lies on extreme edge of P, and therefore T must have q vertices of the form $\lambda_j \mathbf{h}_j$, j = 1, ..., q with each $\lambda_j \geq 1$.

This accounts for all but 3p of the vertices of T. For an $i \in \{1, ..., p\}$, let us say that a vector $(\mathbf{s}, \mathbf{t}, \mathbf{u}, \mathbf{v}) \in \mathbf{R}^{3p+q}$ is x_i -supported if it is zero in all the x_j -coordinates for all $j \in \{1, ..., p\} - \{i\}$. More strongly, say that it is x_i -positive if it is x_i -supported and is positive in at least one of the x_i coordinates. Fix a particular $i \in \{1, ..., p\}$ and consider

the four S-points $\mathbf{r}_i^1, \ldots, \mathbf{r}_i^4$ which are all x_i -positive. Projected into the x_i coordinates, these points are (0, 1/4, 1/2), (1/2, 1/4, 1/2), (1/4, 1/8, 1/2) and (1/4, 3/8, 1/2). Since none of the T-vertices has negative entries, each of $\mathbf{r}_i^1, \ldots, \mathbf{r}_i^4$ must lie in the hull only of T-vertices that are x_i -supported such as $\mathbf{0}, \lambda_1 \mathbf{h}_1, \ldots, \lambda_q \mathbf{h}_q$. Furthermore, it must lie in the hull of at least one x_i -positive vertex of T. In fact, there must be at least three such x_i -positive T-vertices since the four points, when projected into the x_i coordinates, are linearly independent. Thus, T must have at least three x_i -positive vertices for each $i = 1, \ldots, p$. Since there are only 3p vertices of T not yet enumerated, we conclude that T must have exactly three x_i -positive vertices for each i, which we denote $\mathbf{g}_{i,1}, \mathbf{g}_{i,2}, \mathbf{g}_{i,3}$.

Let $\bar{\mathbf{g}}_{i,1}, \bar{\mathbf{g}}_{i,2}, \bar{\mathbf{g}}_{i,3} \in \mathbf{R}^3$ denote the x_i coordinates of $\mathbf{g}_{i,1}, \mathbf{g}_{i,2}, \mathbf{g}_{i,3}$. By the assumption that T covers the four points (0, 1/4, 1/2), (1/2, 1/4, 1/2), (1/4, 1/8, 1/2) and (1/4, 3/8, 1/2) in the projection into the x_i coordinates, we conclude that there must exist a 3×4 matrix B with nonnegative entries such that

$$(\bar{\mathbf{g}}_{i,1}, \bar{\mathbf{g}}_{i,2}, \bar{\mathbf{g}}_{i,3}) \cdot B = \begin{pmatrix} 0 & 1/2 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/8 & 3/8 \\ 1/2 & 1/2 & 1/2 & 1/2 \end{pmatrix}.$$

As mentioned above, all of $\bar{\mathbf{g}}_{i,1}$, $\bar{\mathbf{g}}_{i,2}$, $\bar{\mathbf{g}}_{i,3}$ are nonzero. Because of the inequalities $\mathbf{0} \leq \mathbf{s} \leq \mathbf{u}$ and $\mathbf{0} \leq \mathbf{t} \leq \mathbf{u}$ that define P, it must be the case that the third entries of $\bar{\mathbf{g}}_{i,1}$, $\bar{\mathbf{g}}_{i,2}$, $\bar{\mathbf{g}}_{i,3}$ are all positive and no smaller than the first and second entries. Therefore, define new vectors $\hat{\mathbf{g}}_{i,1}$, $\hat{\mathbf{g}}_{i,2}$, $\hat{\mathbf{g}}_{i,3}$ that are all exactly 1/2 in the last coordinate and have other coordinates lying in [0,1/2] obtained by rescaling each of $\bar{\mathbf{g}}_{i,1}$, $\bar{\mathbf{g}}_{i,2}$, $\bar{\mathbf{g}}_{i,3}$ by twice its third coordinate. By rescaling B in a reciprocal manner, we find that there is a nonnegative matrix \hat{B} such that

$$(\hat{\mathbf{g}}_{i,1}, \hat{\mathbf{g}}_{i,2}, \hat{\mathbf{g}}_{i,3}) \cdot \hat{B} = \begin{pmatrix} 0 & 1/2 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/8 & 3/8 \\ 1/2 & 1/2 & 1/2 & 1/2 \end{pmatrix}.$$

By consider the third row of the above system of equations, we conclude that each column of \hat{B} sums to exactly 1. Then dropping the third row on both sides yields the equation

$$(\hat{\mathbf{g}}_{i,1}(1:2), \hat{\mathbf{g}}_{i,2}(1:2), \hat{\mathbf{g}}_{i,3}(1:2)) \cdot \hat{B} = \begin{pmatrix} 0 & 1/2 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/8 & 3/8 \end{pmatrix},$$

where the notation $\mathbf{v}(1:2)$ denotes the first two entries of a vector. Now we observe that this is precisely a half-sized version of the instance of INTERMEDIATE SIMPLEX described in the preliminary lemma of this section, namely, find three points lying in $[0, 1/2]^2$ whose convex hull covers the four points $\{(0, 1/4), (1/2, 1/4), (1/4, 1/8), (1/4, 3/8)\}$. As established by the lemma, there are precisely two solutions to this system, which we will denote $T_0/2$ and $T_1/2$. Let C_0 be the set of i's such that the triangle defined by $(\hat{\mathbf{g}}_{i,1}(1:2), \hat{\mathbf{g}}_{i,2}(1:2), \hat{\mathbf{g}}_{i,3}(1:2))$ is $T_0/2$, while C_1 is the set of i's such that this triangle is $T_1/2$. Thus we conclude that for $i \in C_0$,

$$(\bar{\mathbf{g}}_{i,1}, \bar{\mathbf{g}}_{i,2}, \bar{\mathbf{g}}_{i,3}) = (\mu_{i,1}(0,0,1), \mu_{i,2}(0,1,1), \mu_{i,3}(1,1/2,1)), \tag{5}$$

and for $i \in C_1$,

$$(\bar{\mathbf{g}}_{i,1}, \bar{\mathbf{g}}_{i,2}, \bar{\mathbf{g}}_{i,3}) = (\mu_{i,1}(1,0,1), \mu_{i,2}(1,1,1), \mu_{i,3}(0,1/2,1)), \tag{6}$$

where $\mu_{i,k} > 0$ for k = 1, 2, 3. This determines the x_i entries of $\mathbf{g}_{i,k}$, k = 1, 2, 3, and the remaining x_j entries are zeros since $\mathbf{g}_{i,k}$ is x_i -positive. Therefore, it remains only to determine the v_j entries of $\mathbf{g}_{i,k}$, k = 1, 2, 3. There are several constraints on these entries as follows. First, we have the inequalities $v_j \geq 0$, and thus all those entries must be nonnegative. Next, we have the constraints $s_i - 2t_i \leq v_j$ whenever $\tilde{x}_i \in c_j$ and $2t_i - 2s_i - u_i \leq v_j$ whenever $x_i \in c_j$. These inequalities are redundant whenever their left-hand side is nonpositive since we have already constrained $v_j \geq 0$. Thus, we need only consider the cases when the left-hand sides are positive. We see that the left-hand side of the first inequality $s_i - 2t_i \leq v_j$ is positive only in the case of $\bar{\mathbf{g}}_{i,1}$ only for $i \in C_1$, and the left-hand side of the second inequality $2t_i - 2s_i - u_i \leq v_j$ is positive only in the case of $\bar{\mathbf{g}}_{i,2}$ only for $i \in C_0$. Thus, for $i \in C_1$, for all j such that \tilde{x}_i occurs as a literal in clause c_j , we must have

$$\mathbf{g}_{i,1}|_{v_i} \ge \mu_{i,1}.\tag{7}$$

(Here, the notation $\mathbf{g}_{i,1}|_{v_j}$ denotes the v_j coordinate entry of $\mathbf{g}_{i,1}$.) Similarly, for $i \in C_0$, for all j such that x_i occurs as a literal in clause c_j , we must have

$$\mathbf{g}_{i,2}|_{v_j} \ge \mu_{i,2}.\tag{8}$$

Next, T must contain the point **b** from (4), so there must be coefficients $\alpha_{i,k}$, $i = 1, \ldots, p$, k = 1, 2, 3 and θ_j , $j = 1, \ldots, q$ adding up to at most 1 and all nonnegative such that

$$\mathbf{b} = \sum_{i=1}^{p} \sum_{k=1}^{3} \alpha_{i,k} \mathbf{g}_{i,k} + \sum_{j=1}^{q} \theta_{j} \lambda_{j} \mathbf{h}_{j}. \tag{9}$$

Fix a particular *i*. The projection of **b** into x_i coordinates is $\bar{\mathbf{b}} = (1/(4p), 1/(4p), 1/(2p))$. Referring back to (5) and (6), one can see that regardless of whether $i \in C_0$ or $i \in C_1$, $\bar{\mathbf{b}}$ is expressed uniquely as $\bar{\mathbf{b}} = \bar{\mathbf{g}}_{i,1}/(8p\mu_{i,1}) + \bar{\mathbf{g}}_{i,2}/(8p\mu_{i,2}) + \bar{\mathbf{g}}_{i,3}/(4p\mu_{i,3})$. Therefore,

$$\alpha_{i,1} = 1/(8p\mu_{i,1}); \quad \alpha_{i,2} = 1/(8p\mu_{i,2}); \quad \alpha_{i,3} = 1/(4p\mu_{i,3}).$$
 (10)

Suppose $i \in C_0$. Then for each j such that x_i occurs as a literal in clause c_j , if we combine (8) and (10), we obtain

$$\left. \sum_{k=1}^{3} \alpha_{i,k} \mathbf{g}_{i,k} \right|_{v_i} \ge 1/(8p).$$

The identical inequality holds when $i \in C_1$ and $\tilde{x}_i \in c_i$.

Now, sum the preceding inequality for i = 1, ..., p to obtain

$$\sum_{i=1}^{p} \sum_{k=1}^{3} \alpha_{i,k} \mathbf{g}_{i,k} \bigg|_{v_j} \ge m_j / (8p), \tag{11}$$

where m_j is the number of literals $x_i \in c_j$ with $i \in C_0$ plus the number of literals $\tilde{x}_i \in c_j$ with $i \in C_1$. Let us now combine these inequalities: From (4), $\mathbf{b}|_{v_j} = 2.5/(8p)$. From (9),

$$\mathbf{b}|_{v_j} \ge \sum_{i=1}^p \sum_{k=1}^3 \alpha_{i,k} \mathbf{g}_{i,k} \bigg|_{v_j},$$

since the last term of (9) is nonnegative. Finally, from (11), the above summation is at least $m_j/(8p)$. Thus, we conclude that $m_j \leq 2.5$. Since m_j is integral, this means $m_j \leq 2$. Let σ be the setting of the x_i 's in the 3-SAT instance defined by taking $x_i = 1$ for $i \in C_1$ and $x_i = 0$ for $i \in C_0$. Then if $x_i \in c_j$ and $i \in C_0$, this literal is falsified in the clause. Similarly, if $\tilde{x}_i \in c_j$ and $i \in C_1$, then this literal is also falsified. In other words, m_j is the number of literals in clause c_j falsified by assignment σ . We have just argued that $m_j \leq 2$ for all $j = 1, \ldots, q$. In other words, for each clause, there are most two literals falsified by assignment σ . Therefore, σ is a satisfying assignment for the 3-SAT instance.

Summarizing, we have proved that if there is a simplex T solving the instance of INTERMEDIATE SIMPLEX, then there are exactly three vertices of T that are x_i -positive for each i = 1, ..., p; that, based on these vertices, i can be classified as either C_0 or C_1 ; and that the assignment σ of the boolean variables in the original 3-SAT instance derived from C_0 and C_1 must be a satisfying assignment.

Conversely, suppose the 3-SAT instance has a satisfying assignment. The vertices of T will be $\mathbf{0}, \lambda_1 \mathbf{h}_1, \ldots, \lambda_q \mathbf{h}_q$ together with $\mathbf{g}_{i,1}, \mathbf{g}_{i,2}, \mathbf{g}_{i,3}$ for each $i=1,\ldots,p$, defined as follows. Let C_0 index the variables set to 0 by the satisfying assignment and C_1 the variables set to 1. Define $\bar{\mathbf{g}}_{i,1}, \bar{\mathbf{g}}_{i,2}, \bar{\mathbf{g}}_{i,3}$ as in (5) and (6) according to C_0 and C_1 . Take $\mu_{i,k} = 5/8$ for all (i,k). (Any other value slightly greater than 1/2 will work.) When $i \in C_0$ and x_i is a literal in c_j , then take $\mathbf{g}_{i,2}|_{v_j} = 5/8$. When $i \in C_1$ and \tilde{x}_i is a literal in c_j , then take $\mathbf{g}_{i,1}|_{v_j} = 5/8$. In all other cases, take $\mathbf{g}_{i,k}|_{v_j} = 0$. It is easy to see that all the inequalities defining P are satisfied by these choices. Furthermore, all the points in S are covered by convex combinations of the 3p + q + 1 points $\mathbf{0}, \lambda_1 \mathbf{h}_1, \ldots, \lambda_q \mathbf{h}_q, \mathbf{g}_{1,1}, \ldots, \mathbf{g}_{p,3}$, which are the vertices of T.

For example, the point $\mathbf{r}_i^1 = (\mathbf{0}, \mathbf{e}_i/4, \mathbf{e}_i/2, \mathbf{e})$ in the case that $i \in C_0$ is expressed as $(2/5)\mathbf{g}_{i,1} + (2/5)\mathbf{g}_{i,2} + \mathbf{h}$, where \mathbf{h} is some linear combination of $\lambda_1\mathbf{h}_1, \ldots, \lambda_q\mathbf{h}_q$ chosen to make the v_j entries each equal to 1. (Note that the v_j entries of $(2/5)\mathbf{g}_{i,1} + (2/5)\mathbf{g}_{i,2}$ before \mathbf{h} is added will be either 0 or 1/4). The total sum of the coefficients to express $(\mathbf{0}, \mathbf{e}_i/4, \mathbf{e}_i/2, \mathbf{e})$ is $2/5 + 2/5 + h_1$, where h_1 is the sum of the coefficients needed in the terms of \mathbf{h} . Select $\lambda_1, \ldots, \lambda_q$ to be large scalars so that we can be assured that $4/5 + h_1 \leq 1$. If this sum is less than 1, then we include a contribution of $\mathbf{0}$, another vertex of T, in the linear combination to make the sum of coefficients exactly 1.

Similarly, as sketched out earlier, to obtain the point $\mathbf{b} = (\mathbf{e}/(4p), \mathbf{e}/(4p), \mathbf{e}/(2p), 2.5\mathbf{e}/(8p))$ in the hull of the vertices of T, we use (9) with coefficients chosen according to (10). This choice of $\alpha_{i,j}$'s yields x_i coordinate entries equal to (1/(4p), 1/(4p), 1/(2p)) for each i and has entries less than or equal to 2/(8p) in each v_j coordinate entry. Then, as above, one can include additional terms involving $\mathbf{0}$ and $\lambda_1 \mathbf{h}_1, \ldots, \lambda_q \mathbf{h}_q$ to complete the convex combination. One point to note is that the sum of the $\alpha_{i,k}$ coefficients appearing in (9), assuming $\mu_{i,k} = 5/8$, is equal to 4/5, and hence does not exceed 1. Addition of the θ_j coefficients will make the total higher but still less than 1 provided $\lambda_1, \ldots, \lambda_q$ are all chosen to be very large.

4 Local-search heuristics

In this section we will prove a theorem about the INTERMEDIATE SIMPLEX problem that will suggest a class of local-search heuristics. The theorem is as follows.

Theorem 5. Consider an instance of INTERMEDIATE SIMPLEX given by polytope $P \subset \mathbf{R}^{k-1}$ with n facets and point set $S \subset P$ with m vectors. Suppose there exists a solution T, and suppose that all vertices of T are given except for one. Then the set of feasible positions for the last vertex is defined by a system of linear equations and inequalities (mk equalities and n + mk inequalities).

Proof. Let the vertices of T be denoted $\mathbf{v}_1, \ldots, \mathbf{v}_k$, and suppose all are known except \mathbf{v}_k . Two sets of constraints must be satisfied, namely, those arising from the requirement $S \subset T$ and those arising from $T \subset P$. Since the simplex T is assumed to be a solution, the given values of $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$ must all lie in P, and hence the constraint on \mathbf{v}_k to ensure that $T \subset P$ is simply that $\mathbf{v}_k \in P$. This clearly amounts to a set of n linear inequalities that must be satisfied by P.

Next, consider the requirement $S \subset T$; choose a particular vector $\mathbf{b} \in S$. If \mathbf{b} is in the hull of $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$ then \mathbf{b} is in T no matter what choice is made for \mathbf{v}_k , so such a \mathbf{b} does not impose any constraint on \mathbf{v}_k . Else suppose \mathbf{b} is not in the hull of $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$. Then the requirement on \mathbf{v}_k is that there exist $\lambda_1, \ldots, \lambda_k$ such that $\lambda_1 \mathbf{v}_1 + \cdots + \lambda_k \mathbf{v}_k = \mathbf{b}$, $\lambda_i \geq 0$, $i = 1, \ldots, k$, and $\lambda_1 + \cdots + \lambda_k = 1$. This constraint is nonlinear because of the product of unknowns $\lambda_k \mathbf{v}_k$. However, we can rearrange it into a linear constraint by dividing through by λ_k (which is nonzero by the hypothesis that \mathbf{b} is not in the hull of $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$) and defining new variables $\alpha_i = \lambda_i/\lambda_k$, $i = 1, \ldots, k-1$, and $\alpha^* = 1/\lambda_k$. Then the above constraints become $\alpha_1 \mathbf{v}_1 + \cdots + \alpha_{k-1} \mathbf{v}_{k-1} + \mathbf{v}_k = \alpha^* \mathbf{b}$, $\alpha_i \geq 0$, $i = 1, \ldots, k-1$, $\alpha^* \geq 0$, $\alpha_1 + \cdots + \alpha_{k-1} + 1 = \alpha^*$, which are all linear. There are k equality constraints and k inequality constraints in this system. A system of this kind is needed for each point in S.

The preceding theorem suggests a local search heuristic for INTERMEDIATE SIM-PLEX. One can choose as an initial guess T a large simplex that contains all of S but perhaps is not contained in P. Then one adjusts the vertices of T one at a time, optimizing a criterion that minimizes departure of the vertex from feasibility. Because the feasible positions for the vertex under consideration form a polyhedron, several possible criteria such as 2-norm distance to feasibility would constitute convex programming problems. Thus, on each iteration of the local search algorithm, one could reposition a single vertex of T optimally until a solution is found.

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References

- [1] Nasimeh Asgarian and Russell Greiner. Using rank-1 biclusters to classify microarray data. Department of Computing Science, and the Alberta Ingenuity Center for Machine Learning, University of Alberta, Edmonton, AB, Canada, T6G2E8, 2006.
- [2] Sven Bergmann, Jan Ihmels, and Naama Barkai. Iterative signature algorithm for the analysis of large-scale gene expression data. *Physical Review E*, 67:031902, 2003.
- [3] M. Biggs, A. Ghodsi, and S. Vavasis. Nonnegative matrix factorization via rank-one downdating. Preprint, 2007.
- [4] L. Blum, F. Cucker, M. Shub, and S. Smale. Complexity of Real Computation. Springer Verlag, 1998.
- [5] J. Cohen and U. Rothblum. Nonnegative ranks, decompositions and factorizations of nonnegative matrices. *Linear Algebra and its Applications*, 190:149–168, 1993.
- [6] J Edmonds. Systems of distinct representatives and linear algebra. *Journal of Research of the National Bureau of Standards*, 71B:241–245, 1967.
- [7] M. R. Garey and D. S. Johnson. Computers and Intractability: A Guide to the Theory of NP-Completeness. W. H. Freeman, 1979.
- [8] Nicolas Gillis. Approximation et sous-approximation de matrices par factorisation positive: algorithmes, complexité et applications. Master's thesis, Université Catholique de Louvain, Louvain-la-Neuve, Belgium, 2006. In French.
- [9] G. H. Golub and C. F. Van Loan. *Matrix Computations, 3rd Edition*. Johns Hopkins University Press, Baltimore, 1996.
- [10] T. Hofmann. Probabilistic latent semantic analysis. In Kathryn B. Laskey and Henri Prade, editors, UAI '99: Proceedings of the Fifteenth Conference on Uncertainty in Artificial Intelligence, Stockholm, Sweden, July 30-August 1, 1999, pages 289–296. Morgan Kaufmann, 1999.
- [11] H. Kim and H. Park. Sparse non-negative matrix factgorizations via alternating non-negativity-constrained least squares for microarray data analysis. Bioinformatics (to appear), 2007.
- [12] D. Lee and H. Seung. Learning the parts of objects by non-negative matrix factorization. *Nature*, 401:788–791, 1999.