EXACT SOLUTIONS IN LOW-RANK APPROXIMATION WITH ZEROS

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Abstract. Low-rank approximation with zeros aims to find a matrix of fixed rank and with a fixed zero pattern that minimizes the Euclidean distance to a given data matrix. We study the critical points of this optimization problem using algebraic tools. In particular, we describe special linear, affine and determinantal relations satisfied by the critical points. We also investigate the number of critical points and how the number is related to the complexity of nonnegative matrix factorization problem.

Key words. Structured low-rank approximation, zero patterns, Euclidean distance degree, nonnegative matrix factorization

AMS subject classifications. 14M12, 14P05, 13P25, 90C26, 68W30

1. Introduction.

The *best rank-r approximation problem* aims to find a rank-r matrix that minimizes the Euclidean distance to a given data matrix. The solution of this problem is completely addressed by the Eckart-Young-Mirsky theorem which states that the best rank-r approximation is given by the first r components of the *singular value decomposition* (SVD) of a real matrix.

We study the *structured best rank-r approximation problem*, namely we consider additional linear constraints on rank-r matrices. We focus on *coordinate subspaces*, i.e., linear spaces that are defined by setting some entries to zero. Let $S \subset [m] \times [n]$ denote the indices of zero entries and let $\mathcal{L}^S$ be the linear subspace of $\mathbb{R}^{m\times n}$ defined by the equations $x_{ij} = 0$ for all $(i,j) \in S$. Given $U = (u_{ij}) \in \mathbb{R}^{m\times n}$, our optimization problem becomes

$$\begin{aligned} &\min_X \, d_U(X) \coloneqq \sum_{i=1}^{m}\sum_{j=1}^{n}(x_{ij}-u_{ij})^2 \\ &\text{s.t. } X \in \mathcal{L}^S \text{ and } \operatorname{rank}(X) \le r\,. \end{aligned} \tag{1.1}$$

Structured low-rank approximation problem has been studied in [CFP03, Mar08, Mar19]. Exact solutions to this problem have been investigated by Golub, Hoffman and Stewart [GHS87], and by Ottaviani, Spaenlehauer and Sturmfels [OSS14]. In [GHS87], rank-r critical points are studied under the constraint that entries in a set of rows or in a set of columns of a matrix stay fixed. This situation is more general than ours in the aspect that the fixed entries are not required to be zero but more restrictive when it comes to the indices of the entries that are fixed. In [OSS14], rank-r critical points restricted to generic subspaces of matrices are studied. In our paper, the linear spaces set some entries equal to zero and hence are not generic. Because of this, we cannot use many powerful tools from algebraic geometry and intersection theory, and we have to come up with algebraic and computational techniques that exploit this special structure. Horobet and Rodriguez study the problem when at least one solution of a certain family of optimization problems satisfies given polynomial conditions, and address the structured low-rank approximation as a particular

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case [HR20, Example 15].

The optimization problem (1.1) is nonconvex and often local methods are used to solve it. They return a local minimum of the optimization problem. There are heuristics for finding a global minimum, but these heuristics do not guarantee that a local minimum is indeed a global minimum. We refer to [Mar08] for various algorithms and to [SS16] for an algorithm with locally quadratic convergence. Cifuentes recently introduced convex relaxations for structured low-rank approximation that under certain assumptions have provable guarantees [Cif19]. Alternatively, the minimization problem (1.1) can be solved globally by looking at all the complex critical points of d_U on

$$\mathcal{L}_r^S \coloneqq \{X \in \mathcal{L}^S \mid \operatorname{rank}(X) \le r\}$$

and selecting the real solution that minimizes the Euclidean distance. If $U \in \mathbb{C}^{m\times n}$ is general, namely if it belongs to the complement of a Zariski closed set, then the number of critical points is constant and is called the *Euclidean Distance degree* (ED degree) of $\mathcal{L}_r^S$. We denote this invariant by $\operatorname{EDdegree}(\mathcal{L}_r^S)$. The importance of the ED degree is that it measures the algebraic complexity of writing the optimal solution as a function of U. More generally, the ED degree of an algebraic variety is introduced in [DHO$^+$16]. The main goal of this paper is to study the critical points and the ED degree of the minimization problem (1.1).

When rank is one, then characterizing critical points becomes a combinatorial problem. More precisely, listing all critical points translates to the problem of listing minimal vertex covers of a bipartite graph. Proposition 3.6 gives the ED degree of $\mathcal{L}_1^S$ in terms of the minimal covers. The complexity of counting vertex covers in a bipartite graph is known to be #P-complete [PB83].

Draisma, Ottaviani and Tocino [DOT18] define the *critical space* of a tensor, a special linear space which contains the linear span of the critical rank-r tensors. For matrices without linear constraints, the critical space coincides with the linear span of the rank-r critical points of d_U (see also [OP15, Section 5]). Our first main result is Theorem 4.5 which studies the linear span of rank-r critical points of d_U in the structured setting. We call it again the *critical space* in the structured setting. More precisely, Theorem 4.5 states that certain linear equations from the unstructured setting in [DOT18, Definition 2.8] are satisfied by the rank-r critical points of d_U in the structured setting. In the unstructured setting, the rank-one critical points form a basis of the critical space and the rank-r critical points are linear combinations of the basis vectors with coefficients in $\{0,1\}$. In the structured setting, there are too few rank-one critical points to give a basis of the critical space. We leave it as an open question, whether there is a natural extension to a basis and whether the coefficients that give rank-r critical points as linear combinations of basis elements, have a nice description.

Our second main result is Proposition 4.13 that describes affine linear relations that are satisfied by the rank-r critical points of d_U in the unstructured setting. In the structured setting, we conjecture the affine linear relations satisfied by the rank-r critical points of d_U. The last kind of constraints satisfied by the rank-r critical points that we consider are nonlinear determinantal constraints given in Proposition 4.19. The ED degree of d_U is studied in Section 5. Our experiments indicate that the ED degree is exponential in $|S|$.

The optimization problem (1.1) is motivated by the *nonnegative matrix factorization* (NMF) problem. Given a nonnegative matrix $X \in \mathbb{R}_{\ge 0}^{m\times n}$, the *nonnegative rank* of X is the smallest r such that

$$X = AB, \text{ where } A \in \mathbb{R}_{\geq 0}^{m\times r} \text{ and } B \in \mathbb{R}_{\geq 0}^{r\times n}.$$

NMF aims to find a matrix X of nonnegative rank at most r that minimizes the Euclidean distance to a given data matrix $U \in \mathbb{R}_{\geq 0}^{m\times n}$.

The nonnegative rank of a nonnegative matrix is always greater or equal than its rank. Cohen and Rothblum show that for a nonnegative matrix of rank at most two, its nonnegative rank equals its rank [CR93]. This implies that the set $\mathcal{M}_2$ of matrices of nonnegative rank at most two is defined by the constraints that the rank of a matrix is at most two and the entries of the matrix are nonnegative. In particular, the rank constraint is equivalent to a set of equations while the nonnegativity constraints are given by inequalities.

To solve the NMF problem with guarantee of finding an optimal solution, we consider all critical points of the Euclidean distance function over $\mathcal{M}_2$. There are two options:

1. A critical point of the Euclidean distance function over $\mathcal{M}_2$ is a critical point of the Euclidean distance function over the set $\mathcal{X}_2$ of matrices of rank at most two.
2. A critical point of the Euclidean distance function over $\mathcal{M}_2$ lies on the boundary of $\mathcal{M}_2$, i.e. the critical point contains one or more zero entries.

Equivalently, the second item gives a critical point of the optimization problem (1.1) for a subset $S \subset [m] \times [n]$. For $r \geq 3$, there are further inequality constraints that are required to characterize the set of matrices of nonnegative rank at most r, see [KRS15] for the inequalities when $r = 3$. Hence there are further critical points in addition to the two types listed above.

In Section 6, we apply the structured best rank-two approximation problem to NMF. We use the ED degree of d_U for different S to show that the number of relevant critical points of the Euclidean distance function over $\mathcal{M}_2$ for 3×3 matrices is 756. For the same case, we show experimentally that the optimal critical point has a few zeros.

The rest of the paper is organized as follows. In Section 2 we set our notations and recall the Eckart-Young-Mirsky Theorem. In Section 3 we address the best rank-one approximation problem with assigned zero patterns. In Section 4 we investigate special polynomial relations among the critical points of d_U. In Section 5 we provide conjectural ED degree formulas for special formats and zero patterns S, obtained from computational experiments. In Section 6 we relate the minimization problem (1.1) to nonnegative matrix factorization. The code for the computations can be found at github.com/kaiekubjas/exact-solutions-in-low-rank-approximation-with-zeros.

2. Preliminaries. We start by setting up the notations used throughout the paper. Without loss of generality, we always assume that $m \leq n$ when considering the vector space $\mathbb{R}^{m\times n}$. Let $\mathcal{X}_r$ denote the variety of $m \times n$ matrices of rank at most r. An important tool to study low-rank approximation problem is given by the following decomposition of a real matrix.

THEOREM 2.1 (Singular Value Decomposition). *Any matrix $U \in \mathbb{R}^{m\times n}$ admits the* Singular Value Decomposition (SVD)

$$U = A\,\Sigma\,B^T\,, \tag{2.1}$$

where $A \in \mathbb{R}^{m\times m}$ and $B \times \mathbb{R}^{n\times n}$ are orthogonal matrices and $\Sigma \in \mathbb{R}^{m\times n}$ is such that $\Sigma_{ii} = \sigma_i$ for some real numbers $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_m \geq 0$, otherwise $\Sigma_{ij} = 0$. The *numbers σ_i are called* singular values *of U. Denoting by a_i and b_i the columns of A and B respectively, for all $i \in [m]$ the pair (a_i, b_i) is called a* singular vector pair *of U. If the singular values are all distinct, then all singular vector pairs are unique up to a simultaneous change of sign.*

Remark 2.2. Theorem 2.1 extends to complex matrices using unitary matrices and their conjugates, but complex conjugation is not an algebraic operation. If we can factor a complex matrix $U \in \mathbb{C}^{m\times n}$ as in (2.1), then U admits an *algebraic SVD*. The complex matrices admitting an algebraic SVD are characterized in [CH87, Theorem 2 and Corollary 3], see also [DLOT17, Section 3].

Since d_U is a polynomial function and $\mathcal{X}_r$ has the structure of an affine variety, the problem of finding all critical points of the function d_U on $\mathcal{X}_r$ can be attacked using algebraic tools. More precisely, a matrix $X \in \mathcal{X}_r$ is a *critical* point of the function d_U if the vector $U - X$ is orthogonal to the tangent space $T_X\mathcal{X}_r$ with respect to the Frobenius inner product. Recall that the *Frobenius inner product* of two $m\times n$ matrices A and B is $\langle A, B\rangle_F \coloneqq \mathrm{trace}(AB^T)$. The following result describes completely all such critical points.

Theorem 2.3 (Eckart-Young-Mirsky). *Consider a matrix $U \in \mathbb{R}^{m\times n}$ of rank k and its SVD as in (2.1). Let $r \in [k]$. Then all the critical points of d_U on $\mathcal{X}_r$ are of the form*

$$A(\Sigma_{i_1} + \cdots + \Sigma_{i_r})B^T$$

for all subsets $\{i_1 < \cdots < i_r\} \subset [k]$, where Σ_j is the $m \times n$ matrix whose only non-zero entry is $\Sigma_{j,j} = \sigma_j$. If the non-zero singular values of U are distinct then the number of critical points is $\binom{k}{r}$.

Therefore, Theorem 2.3 solves the best rank-r approximation problem and the nice structure of critical points leads to various interesting consequences. In particular, assuming that U is full rank, their number is independent from the largest dimension n. Moreover, their linear span does not depend on the rank r; it is studied in [OP15, DOT18] in the more general context of tensor spaces, see also Proposition 4.1.

The following are two basic lemmas needed in the following sections.

Lemma 2.4. *In the Euclidean space $(V, \langle\cdot,\cdot\rangle)$, consider an affine variety $\mathcal{X}$ contained in the proper affine subspace $W \subset V$. Let $\pi_W : V \to W$ be the projection onto V. Then, for all $u \in V$, the critical points on $\mathcal{X}$ of the squared distance functions d_u and $d_{\pi_W(u)}$ coincide.*

Proof. Let $x \in \mathcal{X}$ be a critical point of d_u. In particular $\langle u - x, y\rangle = 0$ for all $y \in T_x\mathcal{X}$. Furthermore $\langle \pi_W(u) - x, y\rangle = \langle u - x, y\rangle - \langle u - \pi_W(u), y\rangle = 0 - 0 = 0$ since $u - \pi_W(u)$ and y sit in orthogonal subspaces. ∎

Lemma 2.5. *In the Euclidean space $(V, \langle\cdot,\cdot\rangle)$, consider affine varieties $\mathcal{X}_1, \ldots, \mathcal{X}_p$ such that $\mathcal{X}_i \not\subset \mathcal{X}_j$ for all $i \neq j$. Then $\mathrm{EDdegree}(\mathcal{X}_1 \cup \cdots \cup \mathcal{X}_p) = \sum_{i=1}^{p} \mathrm{EDdegree}(\mathcal{X}_i)$.*

Proof. The statement follows since, for all $i \in [p]$, a general data point $u \in V$ admits critical points on $\mathcal{X}_i$ outside the singular locus of $\mathcal{X}_1 \cup \cdots \cup \mathcal{X}_p$. ∎

3. Rank-one structured approximation. In this section, we focus on rank-one Euclidean distance minimization in the presence of zeros. We build on the observation that non-zero entries of a rank-one matrix form a rectangular submatrix. Hence, finding the best rank-one approximation with zeros in S consists of three steps:

1. Identify the supports of all maximal rectangular submatrices such that their complement contains the zero pattern S.

2. Find the best rank-one approximation for each of the rectangular supports.
3. Choose the best rank-one approximation over all the supports.

EXAMPLE 3.1. *Let U be an $m \times n$ matrix and $S = \{(1,1)\}$. Finding the best structured rank-one approximate of U requires us to solve the rank-one approximation problem for two rectangular submatrices of sizes $m \times (n-1)$ and $(m-1) \times n$.*

We start by considering two cases for which the structured best rank-r approximation problem with zeros is easy.

Remark 3.2 (Rectangular low-rank approximation). Let $U \in \mathbb{R}^{m \times n}$ and let S be such that the non-zero entries of X form an $m' \times n'$ rectangular submatrix X'. Then solving the structured best rank-r approximation problem (1.1) for X is equivalent to solving the unstructured best rank-r approximation problem for X'. By Theorem 2.3, there are $\binom{m'}{r}$ critical points of d_U and they are given by the Singular Value Decomposition (2.1) of U.

Remark 3.3. Let S be a zero pattern such that the non-zero entries of X form a block diagonal matrix with s blocks. Since the rank of a block diagonal matrix equals the sum of ranks of blocks, consider all partitions of r into s parts. Let r_i denote the size of the i-th part. Then for i-th block consider the critical points of rank-r_i approximation. Taking any possible combination of critical points for each block over all partitions gives all critical points of the original problem.

The main difficulty in studying the best rank-one approximation problem with assigned zero pattern S lies in identifying the supports of all maximal rectangular submatrices such that their complements contain S.

DEFINITION 3.4. *We say that a zero pattern $S \subset [m] \times [n]$ is* rectangular *if the indices that are not in S form a rectangular matrix. More precisely, a rectangular zero pattern has the form $S = (S_1 \times [n]) \cup ([m] \times S_2)$, for some $S_1 \subset [m]$ and $S_2 \subset [n]$. Sometimes we denote this zero pattern also by (S_1, S_2).*

DEFINITION 3.5. *Let $S, T \subset [m] \times [n]$ be two zero patterns.*

1. *The zero pattern T is a* cover *of the zero pattern S, if $S \subset T$ and if T is rectangular.*
2. *The zero pattern T is a* minimal cover *of S, if it is minimal among all covers of the zero pattern S with respect to inclusion. We denote by $MC(S, m, n)$ the set of all minimal covers of $S \subset [m] \times [n]$.*

For example, if $S = \{(1,1), (1,2), (2,2)\}$, then

$$MC(S, 3, 3) = \{([2], \emptyset), (\emptyset, [2]), (\{1\}, \{2\})\}.$$

PROPOSITION 3.6. *Let $S \subset [m] \times [n]$ be a zero pattern. Consider the variety $\mathcal{X}_1$ of $m \times n$ matrices of rank at most one and the intersection $\mathcal{L}_1^S = \mathcal{X}_1 \cap \mathcal{L}^S$. Then*

$$\mathrm{EDdegree}(\mathcal{L}_1^S) = \sum_{(A_r, A_c) \in MC(S,m,n)} \min(m - |A_r|, n - |A_c|).$$

Proof. There is a bijection between the irreducible components of $\mathcal{L}_1^S$ and the elements of $MC(S, m, n)$. More precisely, for every pair $(A_r, A_c) \in MC(S, m, n)$, the corresponding component of $\mathcal{L}_1^S$ is isomorphic to the variety of $(m - |A_r|) \times (n - |A_c|)$ matrices of rank at most one, and by Theorem 2.3 this component has ED degree equal to $\min(m - |A_r|, n - |A_c|)$. Moreover, given two distinct minimal covers in $MC(S, m, n)$, their corresponding irreducible components are not comparable under inclusion. The statement follows by Lemma 2.5. ∎

Definition 3.7. *Two zero patterns S_1 and S_2 are said to be* permutationally equivalent *if there exist permutation matrices P_1 and P_2 such that we can write every element A of $\mathcal{L}^{S_1}$ as $A = P_1 B P_2$ for some $B \in \mathcal{L}^{S_2}$.*

Corollary 3.8. *Let $S \subset [m] \times [n]$ be a zero pattern which is permutationally equivalent to the row zero pattern $\{(1,1), \ldots, (1,|S|)\}$. Then*

$$\mathrm{EDdegree}(\mathcal{L}_1^S) = \min\{m, n - |S|\} + \min\{m-1, n\}\,.$$

Similarly, let $S \subset [m] \times [n]$ be a zero pattern which is permutationally equivalent to the column zero pattern $\{(1,1), \ldots, (|S|,1)\}$. Then

$$\mathrm{EDdegree}(\mathcal{L}_1^S) = \min\{m, n-1\} + \min\{m - |S|, n\}\,.$$

Corollary 3.9. *Let $S \subset [m] \times [n]$ be a zero pattern which is permutationally equivalent to the diagonal zero pattern $\{(1,1), \ldots, (|S|,|S|)\}$. Then*

$$\mathrm{EDdegree}(\mathcal{L}_1^S) = \sum_{j=0}^{|S|} \binom{|S|}{j} \min\{m - j, n - |S| + j\}\,.$$

Enumerating minimal covers of a zero pattern translates to the problem of enumerating minimal vertex covers of a bipartite graph. A bipartite graph G can be associated to a zero pattern of an $m \times n$-matrix $X = (x_{ij})$ in the following way: the bipartite graph G has m and n vertices in the two parts, corresponding to the rows and columns of the matrix. The edges of G correspond to the zero entries of the matrix, i.e. $(i,j) \in E(G)$ if and only if $x_{ij} = 0$. A (minimal) cover of a zero pattern is then equivalent to a (minimal) vertex cover of the corresponding bipartite graph. By König's Theorem, in bipartite graphs the minimum vertex cover problem is equivalent to the maximum matching problem, and it can be solved in polynomial time. However, counting vertex covers in a bipartite graph is #P-complete [PB83].

We suggest Algorithm 3.1, that is based on dynamic programming, to find all minimal covers of a zero pattern S. To simplify notation, we present the algorithm for the bipartite graph G corresponding to the zero pattern S. In particular, we use the following notation. Let $G = (U, V, E)$, where $U = \{u_1, \ldots, u_m\}$ and $V = \{v_1, \ldots, v_n\}$ are the two parts of vertices. For $u \in U$, we denote by $\mathcal{N}(u)$ the set of neighbors of u. Let $U' \subset U$ and $V' \subset V$. We denote by $G[U', V']$ the induced subgraph of G, i.e., the graph whose vertex set is $U' \cup V'$ and whose edge set is the subset of E that consists of edges whose both endpoints are in $U' \cup V'$. We consider the graph $G[U', V']$ as a bipartite graph with U' and V' being the two parts of vertices.

The following example illustrates that it is not enough, even to consider minimal covers with the least number of elements.

Example 3.10. *Consider the 3×4 matrix*

$$U = \begin{pmatrix} 1 & -1 & -2 & -2 \\ 1 & 0 & 1 & -2 \\ 2 & 0 & 0 & 2 \end{pmatrix}.$$

We look for the closest rank-one matrix to U with zero pattern $S = \{(1,1),(1,2)\}$. We have $MC(S,3,4) = \{(\{1\}, \emptyset), (\emptyset, [2])\}$. In particular, the first minimal cover consists of four elements, while the second minimal cover consists of six elements. One verifies that the closest critical point to U is of the second type and is equal to

$$X = \begin{pmatrix} 0 & 0 & -0.627896 & -2.36438 \\ 0 & 0 & -0.430261 & -1.62017 \\ 0 & 0 & 0.496139 & 1.86824 \end{pmatrix}.$$

Algorithm 3.1 Minimal covers of a bipartite graph $G = (U, V, E)$

```
procedure MinimalCovers(G = (U, V, E))
if G is null graph then
    return {(∅, ∅)}
else
    MC = ∅
    MC_1 = MinimalCovers(G[U \ {u_1}, V])
    for (S_1, S_2) ∈ MC_1 do
        append (S_1 ∪ {u_1}, S_2) to MC
    end for
    MC_2 = MinimalCovers(G[U \ {u_1}, V \ N(u_1)])
    for (S_1, S_2) ∈ MC_2 do
        append (S_1, S_2 ∪ N(u_1)) to MC
    end for
    return MC
end if
end procedure
```

4. Special relations among critical points. In this section we provide (some of) the generators of the ideal of critical points on $\mathcal{L}_r^S$ of d_U. In particular, we concentrate on particular linear and affine relations among critical points, and some special nonlinear relations. Some of the results are stated for general linear constraints not necessarily coming from assigned zero patterns.

We first set a few notations. Let X be an $m \times n$ matrix and consider the subsets $I \subset [m]$ and $J \subset [n]$. We always assume that the elements of I and J are ordered in increasing order. We denote by $X_{I,J}$ the submatrix obtained selecting the rows of X with indices in I and the columns of X with indices in J. Moreover, if $|I| = |J|$ we denote by $M_{I,J}(X)$ the minor of X corresponding to rows in I and columns in J. If $I = J = \emptyset$, we set $M_{\emptyset,\emptyset}(X) \coloneqq 1$.

4.1. Linear relations among critical points. Consider a data matrix $U \in \mathbb{R}^{m\times n}$ and let $Z_{U,r}$ be the set of critical points of d_U on $\mathcal{L}_r^S$. We denote by $\langle Z_{U,r}\rangle$ the linear span of $Z_{U,r}$ in $\mathbb{R}^{m\times n}$. A consequence of Theorem 2.3 is that in the unstructured case $\langle Z_{U,r}\rangle = \langle Z_{U,1}\rangle$ for all $r \in [m]$. The following result is a special case of [DOT18, Theorem 1.1] and gives the equations of $\langle Z_{U,r}\rangle$ in the unstructured case.

Proposition 4.1. *Assume $m \le n$ and $S = \emptyset$. Given $U \in \mathbb{R}^{m\times n}$, the subspace $\langle Z_{U,r}\rangle$ has dimension m and is defined by the system*

$$\begin{cases} r_U^{(i,j)} \coloneqq (XU^T - UX^T)_{ij} = 0 \quad \forall\, i,j \in [m] \\ c_U^{(i,j)} \coloneqq (X^TU - U^TX)_{ij} = 0 \quad \forall\, i,j \in [n]\,. \end{cases} \tag{4.1}$$

In particular, the first $\binom{m}{2}$ equations are linearly independent and $m(n-1) - \binom{m}{2}$ equations in the second set are linearly independent. Moreover, no equation of one set is linear combination of equations in the other set.

The study of $\langle Z_{U,r}\rangle$ is more involved when $S \neq \emptyset$. First of all, in the structured setting critical points are not necessarily real: for this reason, we study our problem in $\mathbb{C}^{m\times n}$.

QUESTION 4.2. *If we replace $\mathcal{L}^S$ with a general subspace $\mathcal{L} \subset \mathbb{C}^{m\times n}$, is it true that $\mathcal{L} = \langle Z_{U,r}\rangle$ for every $r \in [m-1]$?*

Small numerical experiments suggest that the answer to Question 4.2 is positive. We show in Theorem 4.5 that the same is not true for $\mathcal{L} = \mathcal{L}^S$ for some zero pattern S.

DEFINITION 4.3. *Let $S \subset [m] \times [n]$ be a zero pattern. We consider the following equivalence relations $\sim_R^S$ and $\sim_C^S$ in the sets $[m]$ and $[n]$, respectively:*

$$\begin{aligned} i \sim_R^S j \quad &\text{if and only if} \quad \chi_S[(i,k)] = \chi_S[(j,k)] \quad \forall k \in [n] \\ i \sim_C^S j \quad &\text{if and only if} \quad \chi_S[(k,i)] = \chi_S[(k,j)] \quad \forall k \in [m]\,, \end{aligned}$$

where χ_S is the characteristic function of S.

DEFINITION 4.4. *We define* critical space *of $U \in \mathbb{R}^{m\times n}$ to be the linear space H_U defined by relations*

$$\left\langle r_U^{(i,j)} \mid i \sim_R^S j \right\rangle + \left\langle c_U^{(i,j)} \mid i \sim_C^S j \right\rangle + \langle x_{ij} \mid (i,j) \in S\rangle\ . \tag{4.2}$$

The previous definition is inspired by [DOT18, Definition 2.8] in the context of unstructured low-rank tensor approximation. Observe that the critical space H_U does not depend on the rank r. If $S = \emptyset$, then $\langle Z_{U,r}\rangle = H_U$ for all $r \in [m-1]$ by Proposition 4.1.

The next result tells that, when passing from unstructured to structured optimization with zero patterns, not all the information about the unstructured critical points is lost.

THEOREM 4.5. *Let $S \subset [m]\times[n]$, $U \in \mathbb{R}^{m\times n}$ and $r \in [m-1]$. Then $\langle Z_{U,r}\rangle \subset H_U$.*

Proof. Let $L_1, \ldots, L_s$ be the constraints that set s entries of the matrix to be equal to zero. We denote by $\mathrm{Jac}_{\mathcal{X}_r}(X)$ and $\mathrm{Jac}_{\mathcal{L}^S}(X)$ the Jacobian matrices of $\mathcal{X}_r$ and $\mathcal{L}^S$ evaluated at X, respectively. The rank-r critical points $X \in \mathcal{L}_r^S$ of d_U satisfy the equality constraints

$$\begin{cases} M_{I,J}(X) = 0 & \forall\, |I| = |J| = r+1 \\ L_k(X) = 0 & \forall\, k \in [s] \end{cases} \qquad \left[\ \lambda \mid \mu \mid 1\ \right] \left[\begin{array}{c} \mathrm{Jac}_{\mathcal{X}_r}(X) \\ \hline \mathrm{Jac}_{\mathcal{L}^S}(X) \\ \hline X - U \end{array}\right] = \left[\ 0 \mid 0 \mid 0\ \right],$$

where $\lambda = (\lambda_{I,J})_{I,J}$ and $\mu = (\mu_1, \ldots, \mu_s)$ are vectors of Lagrange multipliers.

We denote by v the vector of polynomials that is obtained when multiplying the vector and the augmented Jacobian matrix above. Its entries are naturally indexed by $(1,1)$,$\ldots$,(m,n). Let

$$X^{i\leftrightarrow j} := \begin{bmatrix} 0 & \cdots & 0 & -x_{j1} & \cdots & -x_{jn} & 0 & \cdots & 0 & x_{i1} & \cdots & x_{in} & 0 & \cdots & 0 \end{bmatrix}^T$$

be the vector with the entry x_{jk} at the position (i,k) and the entry x_{ik} at the position (j,k) for all $k \in [n]$.

We show that $v \cdot X^{i\leftrightarrow j}$ is equal to a linear constraint in (4.2) plus some $(r+1)$-minors $M_{I,J}(X)$ and linear constraints $L_k(X)$ multiplied with Lagrange multipliers. To do this, we study the products of the rows of the augmented Jacobian with the vector $X^{i\leftrightarrow j}$.

First, observe that the last row of the augmented Jacobian multiplied with $X^{i\leftrightarrow j}$ is precisely the linear form $r_U^{(i,j)}$. Secondly, we show that the rows of the augmented

Jacobian corresponding to minors multiplied with $X^{i\leftrightarrow j}$ are either zero or a sum of $(r+1)$-minors. Let $A = \{a_1, \ldots, a_{r+1}\} \subset [m]$ and $B = \{b_1, \ldots, b_{r+1}\} \subset [n]$. We consider the product

$$\begin{bmatrix} \frac{\partial M_{A,B}(X)}{\partial x_{i1}} & \cdots & \frac{\partial M_{A,B}(X)}{\partial x_{in}} \end{bmatrix} \cdot X^{(j)} . \tag{4.3}$$

If $i \notin A$, then the product (4.3) is equal to zero. Otherwise $i \in A$ and the product (4.3) can be seen as the Laplace expansion of the matrix with rows in $(A \setminus \{i\}) \cup \{j\}$ considered as a multiset and columns in B. Hence if $j \notin A$, then the product (4.3) is equal to the minor corresponding to rows in $(A \setminus \{i\}) \cup \{j\}$ and columns in B. Finally, if $j \in A$, then the product (4.3) is zero again, because the row indexed by j appears twice.

Finally, we consider the rows of the augmented Jacobian corresponding to constraints that $x_{kl} = 0$. The Jacobian of x_{kl} consists of the entry (k,l) being equal to one and all other entries being equal to zero. If $i \neq k$ and $j \neq k$, then the Jacobian of this constraint multiplied by $X^{i\leftrightarrow j}$ is clearly zero. Otherwise the Jacobian of x_{kl} multiplied by $X^{i\leftrightarrow j}$ is either x_{il} of x_{jl}. However both $x_{il} = x_{jl} = 0$ by the assumption $i \sim_R^S j$.

This proves that $r_U^{(i,j)} \in \mathcal{I}(Z_{U,r})$ for all $i \sim_R^S j$. Similarly, one verifies that $c_U^{(i,j)} \in \mathcal{I}(Z_{U,r})$ for all $i \sim_C^S j$ by applying the same argument with the vector

$$X_{i\leftrightarrow j} \coloneqq \begin{bmatrix} -x_{1j} & 0 & \cdots & 0 & x_{1i} & 0 & \cdots & 0 & -x_{nj} & 0 & \cdots & 0 & x_{ni} & 0 & \cdots & 0 \end{bmatrix}^T .$$

∎

The statement of Theorem 4.5 can be adapted to arbitrary linear sections of $\mathcal{X}_r$.

PROPOSITION 4.6. *Let $U \in \mathbb{R}^{m\times n}$. Let $\mathcal{L} \subset \mathbb{C}^{m\times n}$ be the linear subspace defined by the linear forms $L_1, \ldots, L_s$ and let $\langle Z_{U,r}\rangle$ be the linear span of the critical points of d_U on the variety $\mathcal{L}_r$. For all $i < j$, $i,j \in [m]$ and $k \in [s]$, if $\nabla L_k \cdot X^{i\leftrightarrow j} \in \langle L_1, \ldots, L_s\rangle$, then $r_U^{(i,j)} \in \mathcal{I}(Z_{U,r})$. Similarly, for all $i < j$, $i,j \in [n]$ and $k \in [s]$, if $\nabla L_k \cdot X_{i\leftrightarrow j} \in \langle L_1, \ldots, L_s\rangle$, then $c_U^{(i,j)} \in \mathcal{I}(Z_{U,r})$.*

CONJECTURE 4.7. *Let $S \subset [m] \times [n]$, $U \in \mathbb{R}^{m\times n}$ and $r \in [m-1]$. Then $\langle Z_{U,r}\rangle = H_U$ if and only if $\mathcal{L}_r^S$ is irreducible.*

The irreducibility of $\mathcal{L}_r^S$ in Conjecture 4.7 is necessary. In particular, we know from Proposition 3.6 that $\mathcal{L}_1^S$ is never irreducible if $S \neq \emptyset$. We give an example of structured rank-one approximation.

EXAMPLE 4.8 ($m = n = 3$, $r = 1$, $S = \{(1,1)\}$). *In this case, the variety $\mathcal{L}_1^S$ has two irreducible components corresponding to the minimal coverings $(\{1\}, \emptyset)$ and $(\emptyset, \{1\})$. Moreover* $\mathrm{EDdegree}(\mathcal{L}_1^S) = 4$ *by Corollary 3.9. The four critical points on $\mathcal{L}_1^S$ are obtained in this way:*

(i) by computing the SVD of the 3×3 matrix having zero first row and coinciding with U elsewhere (two critical points C_1, C_2),

(ii) by computing the SVD of the 3×3 matrix having zero first column and coinciding with U elsewhere (two critical points C_3, C_4).

One verifies immediately that the critical space H_U is six-dimensional. Therefore $\langle Z_{U,1}\rangle$ is strictly contained in H_U and motivates our hypothesis in Conjecture 4.7.

A higher rank example is showed below.

EXAMPLE 4.9 ($m = n = 3$, $r = 2$, $S = \{(1,1),(1,2)\}$). *The determinant of a 3×3 matrix $X = (x_{ij})$ with zero pattern S is* $\det(X) = x_{13}(x_{21}x_{32} - x_{31}x_{22})$. *Then* *the variety* $\mathcal{L}_2^S$ *has two components* $\mathcal{V}_1 = \mathcal{V}(x_{11}, x_{12}, x_{13})$, $\mathcal{V}_2 = \mathcal{V}(x_{11}, x_{12}, x_{21}x_{32} - x_{31}x_{22})$ *and by Lemma 2.5*

$$\mathrm{EDdegree}(\mathcal{L}_2^S) = \mathrm{EDdegree}(\mathcal{V}_1) + \mathrm{EDdegree}(\mathcal{V}_2) = 1 + 2 = 3\,.$$

The critical point on $\mathcal{V}_1$ *is the projection of* U *onto* $\mathcal{V}_1$. *The two critical points on* $\mathcal{V}_2$ *come by projecting the third column of* U *and computing the SVD of the non-zero* 2×2 *block. In particular, the linear span* $\langle Z_{U,2} \rangle$ *is three-dimensional, whereas the critical space* H_U *has dimension five.*

Corollary 4.10. *Let* $S \subset [m] \times [n]$. *The codimension of* $H_U \subset \mathbb{C}^{m \times n}$ *is*

$$\mathrm{codim}(H_U) = \sum_{C \in [m]/\sim_R^S} \binom{|C|}{2} + \sum_{D \in [n]/\sim_C^S} \gamma_D + |S|,$$

where

$$\gamma_D = \begin{cases} \binom{|D|}{2} & \text{if } |D| \le m \\ m(|D|-1) - \binom{m}{2} & \text{if } |D| \ge m\,. \end{cases}$$

We explain an implication of Proposition 4.1 which is used in the proof of Corollary 4.10.

Remark 4.11. Let $U \in \mathbb{R}^{m \times n}$ and let $U_{I,J}$ be a submatrix of U. Consider the system

$$r_{U_{I,J}}^{(i,j)} = 0 \quad \forall\, i,j \in [|I|]\,,\ c_{U_{I,J}}^{(i,j)} = 0 \quad \forall\, i,j \in [|J|]\,.$$

If $|I| \le |J|$, then the first $\binom{|I|}{2}$ equations are linearly independent. What is more, there are $|I|(|J|-1) - \binom{|I|}{2}$ linearly independent equations in the second set. Finally, no equation in one set is linear combination of equations in the other set.

Proof of Corollary 4.10. We have to show how many of all the linear polynomials appearing in (4.2) are linearly independent.

The first two sets of generators in (4.2) are precisely of the type explained in Remark 4.11. On one hand, since $m \le n$, then $|C| \le n$ for every equivalence class $C \in [m]/\sim_R^S$. This means that all relations $r_U^{(i,j)}$, where $i,j \in C$, are linearly independent. By Remark 4.11 and since equivalence classes on rows are disjoint, this gives in total the first $\sum_{C \in [m]/\sim_R^S} \binom{|C|}{2}$ independent conditions. On the other hand, if $D \in [n]/\sim_C^S$ and $|D| \le m$, then again by Remark 4.11 all relations $c_U^{(i,j)}$, where $i,j \in D$, are linearly independent, thus giving $\binom{|D|}{2}$ independent conditions. Otherwise if $|D| \ge m$, then $m(|D|-1) - \binom{m}{2}$ among the last equations are linearly independent. Since equivalence classes on columns are disjoint, this gives in total the second $\sum_{D \in [n]/\sim_C^S} \gamma_D$ independent conditions. Moreover, again by Remark 4.11, each condition on rows is not a linear combination of equations involving columns, and vice versa.

Finally, consider the last $|S|$ conditions coming from the zero pattern. Trivially each relation x_{ij} is independent from the other variables x_{rs} with $(r,s) \in S$. Moreover, all the conditions $\{x_{ij} \mid (i,j) \in S\}$ are independent from the first two sets of equations because the first two contain no variables with indices in S. ∎

If Conjecture 4.7 is true, then the statement in Corollary 4.10 holds for $\langle Z_{U,r} \rangle$ when $\mathcal{L}_r^S$ is irreducible.

Remark 4.12. Consider again the situation of Example 4.8, but with $r = 2$. By experimental computation, we observe that $\mathrm{EDdegree}(\mathcal{L}_2^S) = 8$ (see Table 2). If linearly independent, the eight critical points should span an eight-dimensional linear space $\langle Z_{U,2}\rangle \subset \mathbb{C}^{3\times 3}$. We verified symbolically using Gröbner bases and elimination that $\mathcal{I}(\langle Z_{U,r}\rangle) = \langle r_U^{(2,3)}, c_U^{(2,3)}, x_{11}\rangle$, thus confirming Conjecture 4.7. In particular $\dim(\langle Z_{U,r}\rangle) = \dim(H_U) = 6$. One might try to extend the basis $\{C_1, C_2, C_3, C_4\}$ of $\langle Z_{U,1}\rangle$ given in Example 4.8 to form a basis of H_U, in the most "natural" way. In this example, we consider the additional two rank-one matrices C_5, C_6 obtained by computing the SVD of the 3×3 matrix having zero first row and column and coinciding with U elsewhere. One might check that the six rank-one matrices $C_1, \ldots, C_6$ are linearly independent and form a basis of H_U.

The matrices C_5 and C_6 are "good" in the sense that they are computed directly from the data matrix U via projections and SVDs. Any critical point $X \in \mathcal{L}_2^S$ may be written as $X = \alpha_1 C_1 + \cdots + \alpha_6 C_6$ for some complex coefficients $\alpha_1, \ldots, \alpha_6$. In Table 1 we display the coefficients α_i of the eight critical points on $\mathcal{L}_2^S$ with respect to the data matrix

$$U = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 2 & 3 \\ 2 & 3 & 4 \end{pmatrix}.$$

	α_1	α_2	α_3	α_4	α_5	α_6
X_1	1.000	1.000	1.000	1.000	-1.000	-1.000
X_2	0.000	1.003	0.000	1.003	-0.000	-0.993
X_3	0.999	-0.024	0.001	-0.024	0.000	0.929
X_4	0.001	-0.024	0.999	-0.024	0.000	0.929
X_5	1.163	$0.500 - 2.994i$	1.163	$0.500 + 2.994i$	-1.347	5.835
X_6	1.163	$0.500 + 2.994i$	1.163	$0.500 - 2.994i$	-1.347	5.835
X_7	$1.082 + 0.127i$	$-1.021 + 2.368i$	$1.082 + 0.127i$	$-1.021 + 2.368i$	$-1.173 - 0.271i$	$-2.455 - 7.814i$
X_8	$1.082 - 0.127i$	$-1.021 - 2.368i$	$1.082 - 0.127i$	$-1.021 - 2.368i$	$-1.173 + 0.271i$	$-2.455 + 7.814i$

TABLE 1
The critical points $X_i \in \mathcal{L}_2^S \subset \mathbb{C}^{3\times 3}$ of d_U in the basis $\{C_1, \ldots, C_6\}$.

More generally, knowing the ideal of critical points $X \in \mathcal{L}_r^S$ for d_U and a basis $\{C_1, \ldots, C_k\}$ of $\langle Z_{U,r}\rangle$ whose elements depend only on U, allows to compute the ideal $\mathcal{J}_\alpha \subset \mathbb{C}[\alpha_1, \ldots, \alpha_k]$ of relations among the coefficients α_i of a representation of X.

This idea needs further investigation and is motivated by the unstructured case. Indeed, given $U \in \mathbb{R}^{m\times n}$, the critical points $C_1, \ldots, C_m$ on $\mathcal{X}_1$ of d_U computed from the SVD of U form a basis of $\langle Z_{U,r}\rangle = H_U$ for any $r \in [m]$. By Theorem 2.3, the critical points on $\mathcal{X}_r$ are written uniquely as $X = \alpha_1 C_1 + \cdots + \alpha_m C_m$ for some coefficients $\alpha_j \in \{0, 1\}$. In this case, the ideal $\mathcal{J}_\alpha$ is zero-dimensional in $\mathbb{C}[\alpha_1, \ldots, \alpha_m]$ and its degree is equal to $\mathrm{EDdegree}(\mathcal{X}_r) = \binom{m}{r}$.

4.2. The affine span of critical points. In the previous section, we regarded structured critical points on $\mathcal{L}_r^S$ as vectors in $\mathbb{C}^{m\times n}$ and studied all linear relations among them. In this section, we look for their affine span. Once more we start from the unstructured case.

PROPOSITION 4.13. *Assume $m = n$ and $S = \emptyset$. Given $U = (u_{ij}) \in \mathbb{R}^{m\times m}$, for every $r \in [m]$ the $\binom{m}{r}$ critical points of d_U on $\mathcal{X}_r$ span an affine hyperplane $W_{U,r} \subset H_U$*

of equation

$$W_{U,r}\colon \sum_{i,j=1}^{m} x_{ij}C_{ij}(U) - r\det(U) = 0\,,$$

where $C_{ij}(U) = (-1)^{i+j}M_{[m]\setminus\{i\},[m]\setminus\{j\}}(U)$ *is the* (i,j)*-th cofactor of* U*.*
In particular, $\{W_{U,r}\}_{r\in[m]}$ *is a finite family of parallel hyperplanes in* H_U*.*

Proof. Let $U\in\mathbb{R}^{m\times m}$, written in SVD form as $U = A\Sigma B^T$. By Theorem 2.3 a critical point $X\in\mathcal{X}_r$ of d_U is of the form $X = A\Sigma_I B^T$ for some $I=\{i_1<\cdots<i_r\}\subset[m]$, where $A=(a_{ij})$, $B=(b_{ij})$ and $\Sigma_I = \operatorname{diag}(0,\ldots,\sigma_{i_1},\ldots,\sigma_{i_r},\ldots,0)$. Therefore X is a linear combination of rank-one critical points with coefficients in $\{0,1\}$. Moreover, the m critical points on $\mathcal{X}_1$ of d_U are linearly independent in H_U. This implies immediately that, for any $r\in[m]$, the $\binom{m}{r}$ critical points on $\mathcal{X}_r$ span an affine hyperplane $W_{U,r}$, and $\{W_{U,r}\}_{r\in[m]}$ is a finite family of parallel hyperplanes in $H_U\cong\mathbb{R}^m$.

It remains to show how to obtain the equation of $W_{U,r}$ in the variables x_{ij}. We do this for $r=1$. The statement follows for general r because a rank-r critical point is a sum of r rank-one critical points. In the following, we apply two times the Cauchy-Binet formula

$$M_{I,J}(PQ) = \sum_{\substack{L\subset[m]\\|L|=|I|}} M_{I,L}(P)M_{L,J}(Q)\quad \forall\, P,Q\in\mathbb{C}^{m\times m}\,.$$

Let $X=(x_{ij}) = A\Sigma_l B^T$ be a rank-one critical point of d_U. In particular, $x_{ij} = \sigma_l\, a_{il}\, b_{jl}$ for all $i,j\in[m]$. Then

$$\begin{aligned}
\sum_{i,j=1}^{m} x_{ij}C_{ij}(U) &= \sigma_l \sum_{i,j=1}^{m} a_{il}\, b_{jl}\, C_{ij}(A\Sigma B^T)\\
&= \sigma_l \sum_{i,j=1}^{m} a_{il}\, b_{jl}\,(-1)^{i+j} \sum_{\substack{L\subset[m]\\|L|=m-1}} M_{\hat{i},L}(A)M_{L,\hat{j}}(\Sigma B^T)\\
&= \sigma_l \sum_{i,j=1}^{m} a_{il}\, b_{jl}\,(-1)^{i+j} \sum_{\substack{L,T\subset[m]\\|L|=|T|=m-1}} M_{\hat{i},L}(A)M_{L,T}(\Sigma)M_{\hat{j},T}(B)\\
&= \sigma_l \sum_{i,j=1}^{m} a_{il}\, b_{jl}\,(-1)^{i+j} \sum_{\substack{L\subset[m]\\|L|=m-1}} M_{\hat{i},L}(A)M_{L,L}(\Sigma)M_{\hat{j},L}(B)\\
&= \sigma_l \sum_{\substack{L\subset[m]\\|L|=m-1}} \prod_{h\in L}\sigma_h \left[\sum_{i=1}^{m}(-1)^{i+l}a_{il}M_{\hat{i},L}(A)\right]\left[\sum_{j=1}^{m}(-1)^{j+l}b_{jl}M_{\hat{j},L}(B)\right]\\
&\overset{(\star)}{=} \sigma_1\cdots\sigma_m \left[\sum_{i=1}^{m}(-1)^{i+l}a_{il}M_{\hat{i},\hat{l}}(A)\right]\left[\sum_{j=1}^{m}(-1)^{j+l}b_{jl}M_{\hat{j},\hat{l}}(B)\right]\\
&= \det(\Sigma)\det(A)\det(B) = \det(U)\,,
\end{aligned}$$

where $\hat{i} = [m]\setminus\{i\}$ and identity $(\star)$ holds because the only subset L giving a non-zero summand is $L=\hat{l}$. ∎

The following corollary generalizes Proposition 4.13 to non-squared case.

COROLLARY 4.14. *Given $U \in \mathbb{R}^{m\times n}$ $(m \le n)$, the $\binom{m}{r}$ critical points of d_U on $\mathcal{X}_r$ span an affine hyperplane $W_{U,r} \subset H_U$ of equation*

$$W_{U,r}\colon \sum_{i,j=1}^{m} (X_I)_{ij} C_{ij}(U_{[m],I}) - r\det(U_{[m],I}) = 0\,,$$

where $I = \{i_1 < \cdots < i_m\} \subset [n]$ and, modulo the ideal $\mathcal{I}(H_U)$, the above equation does not depend on the particular choice of I.

In the next example we observe which of the affine relations of Corollary 4.14 still hold true in the structured case.

EXAMPLE 4.15. *Let $U \in \mathbb{R}^{3\times 4}$. In this example we investigate the best rank-two approximation of U with zero pattern $S = \{(1,1)\}$. By experimental computation, we observe that* $\mathrm{EDdegree}(\mathcal{L}_r^S) = 8$. *The eight critical points of d_U span a seven-dimensional linear space $\langle Z_{U,2}\rangle = H_U$ whose ideal is*

$$\mathcal{I}(H_U) = \langle r_U^{(2,3)}, c_U^{(2,3)}, c_U^{(2,4)}, c_U^{(3,4)}, x_{11}\rangle\,.$$

Moreover, the critical points satisfy the affine relation in H_U

$$\sum_{i,j=1}^{3} (X_I)_{ij} C_{ij}(U_{[3],I}) - 2\det(U_{[3],I}) = 0 \text{ for } I = \{2,3,4\}\,.$$

The previous example motivates the following conjecture in structured setting.

CONJECTURE 4.16. *Assume that $\mathcal{L}_r^S$ is irreducible. Given a subset $I \subset [n]$ with $|I| = m$, the complex critical points of d_U on $\mathcal{L}_r^S$ satisfy the additional affine relation*

$$\sum_{i,j=1}^{m} (X_{[m],I})_{ij} C_{ij}(U_{[m],I}) - r\det(U_{[m],I}) = 0 \tag{4.4}$$

if any only if $S \cap ([m]\times I) = \emptyset$.

Conjecture 4.16 is not valid if $\mathcal{L}_r^S$ is not irreducible, as showed in the next example.

EXAMPLE 4.17 $(m = n = 3,\ r = 2,\ S = \{(1,1),(1,2)\})$. *Following up Example 4.9, we observe that the ideal of affine relations among the critical points is*

$$\left\langle r_U^{(2,3)}, c_U^{(1,2)}, x_{11}, x_{12}, x_{23}-u_{23}, x_{33}-u_{33}, \sum_{i,j=1}^{3} \widetilde{X}_{ij} C_{ij}(\widetilde{U}) - 2\det(\widetilde{U})\right\rangle\,, \tag{4.5}$$

where the matrices $\widetilde{U}$ and $\widetilde{X}$ coincide with U and X outside S, respectively, and are zero otherwise. The seven affine relations are independent and thus define an affine plane in $\mathbb{C}^{3\times 3}$.

The first four relations are linear and define the critical space H_U. The last affine relation in (4.5) is equivalent to $\sum_{i,j=1}^{3} x_{ij}C_{ij}(U) - r\det(U) = 0$ modulo $\mathcal{I}(\mathcal{L}^S) = \langle x_{11}, x_{12}\rangle$, since by Lemma 2.4 the matrix U shares the same critical points of its projection $\pi_{\mathcal{L}^S}(U)$ onto $\mathcal{L}^S$. On one hand, this affine relation coincides with (4.4) for $I = J = [3]$. On the other hand, in this case $S \cap ([3]\times[3]) \neq \emptyset$.

4.3. Special nonlinear relations among structured critical points. In Section 4.1, we observed that the special linear constraints $\mathcal{L}^S$ coming from zero patterns $S \subset [m]\times[n]$ preserve some of the linear relations among unstructured critical points. In this subsection, we deal with special nonlinear relations among unstructured or structured critical points. The following is a consequence of [DHO+16, Theorem 5.2] and Theorem 2.3.

PROPOSITION 4.18. *Let $U \in \mathbb{R}^{m\times n}$. Every critical point $X \in \mathcal{X}_r$ of d_U is such that $U - X \in \mathcal{X}_r^\vee = \mathcal{X}_{m-r}$ and $U - X$ is a critical point of d_U as well. In particular, for every subset $A \subset [m]$ and $B \subset [n]$ with $|A| = |B| \geq m - r + 1$, we have that*

$$M_{A,B}(U - X) = 0\,. \tag{4.6}$$

The main result of this subsection is the next proposition which states that some of the relations in (4.6) hold even in the structured case.

PROPOSITION 4.19. *Let $S \subset [m] \times [n]$, $U \in \mathbb{R}^{m\times n}$ and consider a critical point $X = (x_{ij}) \in \mathcal{L}_r^S$ of d_U. Let $A \times B \subset [m] \times [n]$ with $|A| = |B| \geq m - r + 1$ and such that $S \cap (A \times B) = 0$. Then $M_{A,B}(U - X) = 0$.*

Proof. In the following, we denote by $L_1, \ldots, L_{|S|}$ the constraints that set the entries in $S \subset [m] \times [n]$ of the structured matrices to be equal to zero. We recall from Theorem 4.5 that the critical points $X = (x_{ij}) \in \mathcal{L}_r^S$ of d_U are the solutions of the system

$$\begin{cases} M_{I,J}(X) = 0 & \forall\, |I| = |J| = r + 1\\ L_k(X) = 0 & \forall\, k \in [|S|]\\ u_{ij} - x_{ij} = \sum_{I,J} \frac{\partial M_{I,J}}{\partial x_{ij}}\lambda_{I,J} + \sum_{k=1}^{t} \frac{\partial L_k}{\partial x_{ij}}\mu_k & \forall\, (i,j) \in [m] \times [n]\,. \end{cases} \tag{4.7}$$

Let $A\times B \subset [m]\times[n]$ with $|A| = |B| = s$ and assume $S\cap(A\times B) = 0$. Equivalently we have $\frac{\partial L_k}{\partial x_{ij}} = 0$ for all $k \in [t]$ and for all $(i, j) \in A \times B$. Define the matrix

$$\partial(f) \coloneqq \left(\frac{\partial f}{\partial x_{ij}}\right) \in \mathbb{C}^{m\times n} \quad \forall\, f = f(x_{ij}) \in \mathbb{C}[x_{ij}]\,.$$

Using the third set of equations in (4.7), we get the identity

$$M_{A,B}(U - X) = M_{A,B}\left(\sum_{I,J} \partial(M_{I,J}(X))\lambda_{I,J}\right) =: F_{A,B}. \tag{4.8}$$

Under the assumption $S \cap (A \times B) = 0$, the polynomial $F_{A,B}$ does not depend on the linear constraints $L_k(X) = 0$, and thus it is independent of S. Hence the equality (4.8) for $S = \emptyset$ involves the same $F_{A,B}$ as for any other S satisfying $S\cap(A\times B) = 0$. By Proposition 4.18, $M_{A,B}(U - X) = 0$ in the unstructured case, and hence $M_{A,B}(U - X) = 0$ in the structured case. ∎

Remark 4.20. The polynomial $F_{A,B}$ is homogeneous in the $\ell_{I,J}$'s and all coefficients of the monomials of $F_{A,B}$ in the $\ell_{I,J}$'s belong to $\mathcal{I}(\mathcal{X}_r)$ for all $A\times B \subset [m]\times[n]$ with $s \geq m - r + 1$.

Remark 4.21. The condition $S\cap(A\times B) = 0$ in Proposition 4.19 is sufficient but not necessary to prove that $M_{A,B}(U - X) = 0$. For example, let $m = n = 3$, $r = 2$,

$s = 1$ and $S = \{(1,1)\}$. If $A = B = [3]$, we obtain that (here $\lambda_{[3],[3]} = \lambda$, $\mu_1 = \mu$ and $M_{[3],[3]}(X) = \det(X)$)

$$F_{[3],[3]} = \det(X)^2\lambda^3 + x_{11}\det(X)\lambda^2\mu\,,$$

that is, $F_{[3],[3]} \in \mathcal{I}(\mathcal{X}_2)$ and consequently $\det(U - X) = 0$.

The statement of Proposition 4.19 can be generalized to arbitrary linear sections $\mathcal{L}_r$ of $\mathcal{X}_r$. The condition which replaces $S \cap (A \times B) = 0$ is simply that $\frac{\partial L}{\partial x_{ij}} = 0$ for all $L \in \mathcal{I}(\mathcal{L})$, namely no linear constraint depends by variables x_{ij} with indices in $A \times B$. Again this condition is far from being necessary. To show this, below we restrict to one constraint $L = \sum_{i,j} v_{ij}x_{ij}$ and to the variety of corank one square matrices $\mathcal{X}_{m-1} \subset \mathbb{C}^{m\times m}$. We prove that the rank of $U - X$ is completely characterized by the rank of the coefficient matrix $V = (v_{ij})$.

Proposition 4.22. *Consider a linear form* $L = \sum_{i,j=1}^m v_{ij}x_{ij}$ *for some matrix* $V = (v_{ij}) \in \mathbb{C}^{m\times m}$. *Let* $U \in \mathbb{R}^{m\times m}$ *and let* $X \in \mathcal{L}_{m-1} = \mathcal{X}_{m-1} \cap \mathcal{V}(L)$ *be a critical point of* d_U. *Then for all* $2 \le k \le m$

$$\mathrm{rk}(U - X) \le k - 1 \textit{ if and only if } \mathrm{rank}(V) \le k - 2\,.$$

In particular $\mathrm{rank}(U - X) \ge 1$ *if* $V \neq 0$ *and* $\mathrm{rank}(U - X) = 1$ *if and only if* $V = 0$, *namely in the unstructured case.*

Proof. Recall the notation introduced at the beginning of Section 4. We have $\mathcal{I}(\mathcal{L}_{m-1}) = \langle \det(X), L\rangle$. Suppose that $\mathrm{rk}(U - X) \le k - 1$, namely $M_{A,B}(U - X) = 0$ for all $A, B \subset [m]$ with $|A| = |B| = k$. Using the system (4.7) we get that

$$M_{A,B}(U - X) = M_{A,B}(\lambda\partial(\det(X)) + \mu\partial(L)) = M_{A,B}(\lambda C(X) + \mu V)\,, \tag{4.9}$$

where $C(X) = (C_{ij}(X))$ is the cofactor matrix of X. Assume $A = B = [k]$. Our goal is to expand the polynomial at the right-hand side of (4.9), which we call G_k for brevity. First, we consider the following expansion of $M_{[k],[k]}(P + Q)$ for all $P, Q \in \mathbb{C}^{m\times m}$:

$$M_{[k],[k]}(P + Q) = \sum_{\substack{I,J\subset[k]\\|I|=|J|}} (-1)^{I+J} M_{I,J}(P) M_{[k]\setminus I,[k]\setminus J}(Q)\,,$$

where $(-1)^{I+J} = (-1)^{\sum_{i\in I} i + \sum_{j\in J} j}$. This identity follows from the Laplace expansion of the determinant in multiple columns, that can be found for example in [CSS13, Lemma $A.1(f)$]. We apply it in the case $P = \lambda C(X)$ and $Q = \mu V$:

$$G_k = \sum_{\substack{I,J\subset[k]\\|I|=|J|}} (-1)^{I+J} M_{I,J}(C(X)) M_{[k]\setminus I,[k]\setminus J}(V)\,\lambda^{|I|}\mu^{k-|I|}\,.$$

Then we apply the identity

$$M_{I,J}(C(X)) = \begin{cases} 1 & \text{if } I = J = \emptyset \\ (-1)^{I+J}\det(X)^{|I|-1} M_{[k]\setminus I,[k]\setminus J}(X) & \text{if } |I| = |J| \ge 1 \end{cases}$$

which follows from the relation $C(X) = \det(X)\,X^{-T}$ and the *Jacobi complementary minor Theorem*, see [Lal96] and [CSS13, Lemma $A.1(e)$]. Hence we get

$$G_k = M_{[k],[k]}(V)\mu^k + \sum_{\substack{I,J\subset[k]\\|I|=|J|\ge 1}} \det(X)^{|I|-1} M_{[k]\setminus I,[k]\setminus J}(X) M_{[k]\setminus I,[k]\setminus J}(V)\,\lambda^{|I|}\mu^{k-|I|}\,.$$

Finally, using the condition $\det(X)=0$, the previous identity simplifies to

$$G_k = M_{[k],[k]}(C)\mu^k + \sum_{i,j\in[k]} M_{[k]\setminus\{i\},[k]\setminus\{j\}}(X)M_{[k]\setminus\{i\},[k]\setminus\{j\}}(V)\,\lambda\mu^{k-1}\,.$$

Similarly, for arbitrary $A,B\subset[m]$ with $|A|=|B|=k$, we get that

$$M_{A,B}(U-X) = M_{A,B}(C)\mu^k + \sum_{i\in A,j\in B} M_{A\setminus\{i\},B\setminus\{j\}}(X)M_{A\setminus\{i\},B\setminus\{j\}}(V)\,\lambda\mu^{k-1}\,.$$

The consequence is that a critical point X of d_U is such that $\mathrm{rank}(U-X)\le k-1$ if and only if $M_{A\setminus\{i\},B\setminus\{j\}}(V)=0$ for all $i\in A$, $j\in B$ and $A,B\subset[m]$ with $|A|=|B|=k$, or equivalently $\mathrm{rank}(V)\le k-2$. ∎

The main observation coming from Proposition 4.22 is that a general linear constraint L destroys the structure of critical points coming from Theorem 2.3, in particular the relations $M_{A,B}(U-X)$ for suitable A and B. However, if L is special, these conditions might still hold, even in the case when L involves entries x_{ij} with $(i,j)\in A\times B$.

5. Computations of Euclidean Distance degrees. In this section we present various experiments that study the ED degree of $\mathcal{L}_r^S$, when $r\ge 2$ and the zero pattern S involves only elements in the diagonal.

First, we restrict to square matrices and consider the zero pattern $S=\{(1,1)\}$. Since the number of (complex) critical points of d_U on $\mathcal{L}_{n-1}^S$ is constant for a general (complex) data matrix U, it is reasonable to apply a monodromy technique for computing these critical points numerically. For this, we use a `Julia` package `HomotopyContinuation.jl` [BT18]. The number of solutions obtained (that is, the ED degree of $\mathcal{L}_{n-1}^S$ with respect to the Frobenius inner product) is reported in Table 2.

n	3	4	5	6	7	8	9	10
EDdegree($\mathcal{L}_{n-1}^S$)	8	13	18	23	28	33	38	43

TABLE 2
ED degrees for $n\times n$ matrices of rank $\le n-1$ *and* $S=\{(1,1)\}$.

Our experimental results support the following conjecture.

CONJECTURE 5.1. *Consider the variety $\mathcal{L}_{n-1}^S\subset\mathbb{C}^{n\times n}$, where $S=\{(1,1)\}$. Then*

$$\mathrm{EDdegree}(\mathcal{L}_{n-1}^S) = 5(n-1)-2\,.$$

Next, we fix the diagonal zero pattern $S=\{(1,1),\dots,(s,s)\}$ for $s\in[4]$, and we consider the variety $\mathcal{L}_2^S\subset\mathbb{C}^{m\times n}$. We present in Tables 3,4,5,6 the values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ computed depending on the format $m\times n$. Our experiments support the following conjectural formulas.

CONJECTURE 5.2. *Consider the variety $\mathcal{L}_2^S\subset\mathbb{C}^{m\times n}$ with respect to the zero pattern $S=\{(1,1),\dots,(s,s)\}$ for $s\in[4]$. Let $l=\min(m,n)$. Then*

$$\mathrm{EDdegree}(\mathcal{L}_2^S) = \begin{cases} 3(l-1)^2-2(l-1) & \text{if } s=1\\ 18(l-2)^2+6(l-2)+1 & \text{if } s=2 \text{ and } m\neq n\\ 18(l-2)^2+10(l-2)+1 & \text{if } s=2 \text{ and } m=n\\ 108(m-3)^2+144(m-3)+30 & \text{if } s=3 \text{ and } m=n\\ 648(m-4)^2+1600(m-4)+488 & \text{if } s=4 \text{ and } m=n\,. \end{cases}$$

$s \backslash n$	3	4	5	6	7	8	9	10	11	12
3	8	8	8	8	8	8	8	8	8	8
4	8	21	21	21	21	21	21	21	21	21
5	8	21	40	40	40	40	40	40	40	40
6	8	21	40	65	65	65	65	65	65	65
7	8	21	40	65	96	96	96	96	96	96
8	8	21	40	65	96	133	133	133	133	133
9	8	21	40	65	96	133	176	176	176	176
10	8	21	40	65	96	133	176	225	225	225
11	8	21	40	65	96	133	176	225	280	280
12	8	21	40	65	96	133	176	225	280	341

TABLE 3
Values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ *for* $S = \{(1,1)\}$.

$s \backslash n$	3	4	5	6	7	8	9	10	11	12
3	25	29	29	29	29	29	29	29	29	29
4	29	85	93	93	93	93	93	93	93	93
5	29	93	181	193	193	193	193	193	193	193
6	29	93	193	313	329	329	329	329	329	329
7	29	93	193	329	481	501	501	501	501	501

TABLE 4
Values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ *for* $S = \{(1,1),(2,2)\}$.

Remark 5.3. The values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ in Table 3 are known as *octagonal numbers*: writing $0,1,2,\dots$ in a hexagonal spiral around 0, then these are numbers on the line starting from 0 and going in the direction of 1 [Slo, A000567]. Also the diagonal entries of Table 4 form another interesting integer sequence, see [Slo, A081272].

Our experiments suggest a formula for $\mathrm{EDdegree}(\mathcal{L}_2^S)$ in the square case.

CONJECTURE 5.4. *Consider the variety* $\mathcal{L}_2^S \subset \mathbb{C}^{m\times m}$*, where* S *is the zero pattern* $\{(1,1),\dots,(s,s)\}$ *for some* $s \geq 2$*. Then for some constant* c

$$\mathrm{EDdegree}(\mathcal{L}_2^S) = 3^s\, 2^{s-1}(n-s)^2 + s^{s-1}(s+1)^{\lceil s/2\rceil}(n-s) + c\,.$$

Remark 5.5. In Tables 3,4,5,6 we observe the following symmetry property for the variety $\mathcal{L}_r^S \subset \mathbb{C}^{m\times n}$, where $S = \{(1,1),\dots,(s,s)\}$ for some $s \geq 2$:

$$\mathrm{EDdegree}(\mathcal{L}_r^S)(m,n,r,s) = \mathrm{EDdegree}(\mathcal{L}_r^S)(n,m,r,s)\,.$$

This identity always holds, because the two structured best rank-r approximation problems are the same after relabeling variables.

We conclude by performing the same experiments showed at the beginning of the section, but restricting our study to the subspace $\mathrm{Sym}_n(\mathbb{C}) \subset \mathbb{C}^{n\times n}$ of $n\times n$ symmetric matrices. We denote again by $\mathcal{L}_2^S$ the variety of symmetric matrices of rank at most 2 with (symmetric) zero pattern $S \subset [n]\times[n]$. The values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ with respect to the diagonal zero pattern $S = \{(1,1),\dots,(s,s)\}$ are reported in Table 7.

$s \backslash n$	3	4	5	6	7
3	30	62	66	66	66
4	62	282	358	366	366
5	66	358	750	870	882
6	66	366	870	1434	1598
7	66	366	882	1598	2334

TABLE 5
Values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ *for* $S = \{(1,1),(2,2),(3,3)\}$.

$s \backslash n$	4	5	6	7	8
4	488	968	1072	1080	1080
5	968	2736	?	?	?

TABLE 6
Values of $\mathrm{EDdegree}(\mathcal{L}_2^S)$ *for* $S = \{(1,1),(2,2),(3,3),(4,4)\}$.

CONJECTURE 5.6. *Consider the variety* $\mathcal{L}_2^S \subset \mathrm{Sym}_n(\mathbb{C})$*, where* S *is the zero pattern* $\{(1,1),\ldots,(s,s)\}$ *for all* $s \in [4]$*. Then*

$$\mathrm{EDdegree}(\mathcal{L}_2^S) = \begin{cases} 3(n-1)-2 & \text{if } s=1 \\ 9(n-2)-2 & \text{if } s=2 \\ 27(n-3)+4 & \text{if } s=3 \\ 81(n-4)+28 & \text{if } s=4\,. \end{cases}$$

6. Nonnegative low-rank matrix approximation. In this section, we apply rank-two approximation with zeros to the problem of nonnegative rank-two approximation. Our goal is to find the best nonnegative rank-two approximate with a guarantee that we have found the correct solution. We recall that there are two options for the critical points of the Euclidean distance function over $\mathcal{M}_2$:

1. A critical point of the Euclidean distance function over $\mathcal{M}_2$ is a critical point of the Euclidean distance function over the set $\mathcal{X}_2$ of matrices of rank at most two.
2. A critical point of the Euclidean distance function over $\mathcal{M}_2$ lies on the boundary of $\mathcal{M}_2$, i.e. the critical point contains one or more zero entries.

In Example 6.2, we consider 3×3 matrices and show that computing the Euclidean distance to 756 points guarantees finding the best nonnegative rank-two approximate. This example together with the ED degree computations in Section 5 suggests that the exact nonnegative rank-two approximation problem is highly nontrivial, although in general problems on nonnegative decompositions tend to be easier for decompositions of size at most 2 or 3.

Recall, that for a $m\times n$ matrix M there is an algorithm for nonnegative factorization with complexity $O((mn)^{O(r^2 2^r)})$, where r is the nonnegative rank [AGKM16], see also [Moi16]. We can also compute a rank r approximate nonnegative factorization, under the Frobenius norm $\|M\|_F$, in $2^{\mathrm{poly}(r \lg(1/\epsilon))}$ with relative error $O(\epsilon^{1/2} r^{1/4})$ [AGKM16]. We notice that both algorithms run in polynomial time when the rank is fixed. Nevertheless, their implementation is far from straightforward and the exact constants hidden in the big-O notation could be rather big.

$s \backslash n$	2	3	4	5	6	7	8	9	10
1	1	4	7	10	13	16	19	22	25
2	1	7	16	25	34	43	52	61	70
3		4	31	58	85	112	139	166	193
4			28	109	190	271	352	433	514

TABLE 7
Values of $\mathrm{EDdegree}(\mathcal{L}_2^S) \subset \mathrm{Sym}_n(\mathbb{C})$ *for* $S = \{(1,1), \ldots, (s,s)\}$.

We end this section with simulations demonstrating that most of the time, the optimal solution is given by a critical point with a few zeros. The reader might wonder whether it is interesting to consider the 3×3 case, when in practical applications much larger matrices are considered. We believe that thoroughly understanding small cases is important for understanding the structure of the problem, and might provide insights for developing better numerical algorithms.

In the following example, we demonstrate that in the case of 3×3-matrices, the critical points of the rank-two approximation with zeros can be often described explicitly.

EXAMPLE 6.1. *Let* $U = (u_{ij}) \in \mathbb{R}^{3\times 3}$. *We consider the best rank-two approximation problem with zeros in* $S = \{(1,1),(1,2),(2,2)\}$. *Then there are three critical points, each of which has in addition to the entries in* S *one further entry equal to zero and all other entries are equal to the corresponding entries of the matrix* U. *Specifically, the critical points are*

$$\begin{pmatrix} 0 & 0 & 0 \\ u_{21} & 0 & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & u_{13} \\ 0 & 0 & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & u_{13} \\ u_{21} & 0 & u_{23} \\ u_{31} & 0 & u_{33} \end{pmatrix}.$$

The additional entries that are set to zero can be read from the determinant of the matrix

$$\begin{pmatrix} 0 & 0 & x_{13} \\ x_{21} & 0 & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix},$$

that is $x_{13}x_{21}x_{32}$. *Its factors correspond precisely to the additional entries that are set to zero to obtain the three critical points.*

In other words, we consider the Euclidean distance minimization problem to the variety defined by $x_{13}x_{21}x_{32}$. *Since this variety is reducible, we can consider the Euclidean distance minimization problem to each of its three irreducible components. Each of the irreducible components has ED degree 1.*

This example generalizes to $n \times n$ *matrices whose non-zero entries form a lower triangular submatrix. The determinant of such a matrix is the product of the diagonal elements, and hence the critical points of the best rank* $(n-1)$*-approximation problem are obtained by adding a zero to the diagonal.*

A more interesting example is given when $S = \{(1,1),(1,2)\}$. *In this case, the determinant is* $x_{13}(-x_{22}x_{31} + x_{21}x_{32})$. *One of the critical points has the entry* x_{13} *equal to zero and other entries equal to the corresponding entries of* U. *The two other critical points agree with* U *in the third column and the* 2×2 *submatrix defined by the rows* $2,3$ *and columns* $1,2$ *is equal to one of the critical points of the rank-one approximation for the corresponding* 2×2 *submatrix of* U.

This example generalizes to a zero pattern that contains all but one entry in a row *or in a column. Then the determinant factors as a variable times a* $(n-1)\times(n-1)$ *subdeterminant. One critical point is obtained by adding the missing zero and the rest of the critical points are obtained by rank* $(n-2)$*-approximations for the* $(n-1)\times(n-1)$ *submatrix whose determinant is a factor in the above product.*

In the following example, we discuss how to find the best nonnegative rank-two estimate of a 3×3-nonnegative matrix with guarantee.

Example 6.2. *Consider the group whose elements are simultaneous permutations of rows and columns of a* 3×3 *matrix, and permutations of rows with columns. This group acts on the set zero patterns of a* 3×3 *matrix. There are* 26 *orbits of this group action,* 13 *of which are listed in Table 8. The columns of Table 8 list an orbit representative, the orbit size, the ED degree and the description of critical points if available.*

The 13 *orbit representatives listed in Table 8 have the property that there is no zero pattern* S *with less zeros such that the zero pattern of a critical point for* S *is contained in the orbit representative. For example, no zero pattern that contains a row or a column is listed in Table 8, because a critical point on the line three of the table has a row of zeros. If a critical point agrees with* U *at all its non-zero entries, then adding more zeros causes the Euclidean distance to the data matrix to increase, so such critical points can be discarded.*

Moreover, we can also discard the seven orbits of zero patterns marked with star in Table 8, because their critical points either appear earlier in the table or the zero patterns of critical points contain the zero pattern of a critical point that appears earlier in the table.

In summary, there are five different kinds of critical points to be considered:

1. *Sum of any 2 components of the SVD of* U*. In total:* $1\cdot 3=3$.
2. *Critical points of diagonal zero patterns. In total:* $9\cdot 8+18\cdot 25+6\cdot 30=702$.
3. *Critical points that set one row or column of* U *to zero. In total:* $6\cdot 1=6$.
4. *Critical points where a* 2×2*-submatrix is given by a rank-one critical point of the corresponding submatrix of* U*. These critical points also have two zeros and one row or column equal to the corresponding row or column of* U*. In total:* $18\cdot 2=36$.
5. *Critical points where zeros form a* 2×2*-submatrix. In total:* $9\cdot 1=9$.

In total, the number of critical points is $3+702+6+36+9=756$*. Thus, given a nonnegative* 3×3*-matrix* U*, if we construct the* 756 *critical points described above and choose among the nonnegative critical points the one that is closest to* U*, then it is guaranteed to be the best nonnegative rank-two approximation of the matrix* U*.*

Example 6.2 suggests that finding the best nonnegative rank-two approximation of a general matrix with guarantee might be hopeless, because we expect the number of critical points to increase at least exponentially in the matrix size by the conjectures in Section 5. In practice, the best rank-two approximation often has a few zeros.

Using `Macaulay2` [GS] we sampled uniformly randomly 10^5 matrices from the set of 3×3 matrices with real nonnegative entries and the sum of entries being equal to 1000. In 88561 cases, the best approximation has no zeros; in 10550 cases, the best approximation has one zero; in 889 cases, the best approximation has two zeros in different rows and columns. Based on this experiment, we observed two interesting phenomena:

(*a*) We never encountered a best nonnegative rank-two approximation with three zeros or with two aligned zeros.

(*b*) If the best nonnegative rank-two approximation has zero pattern S, then the

	S	#orbit	EDdegree($\mathcal{L}_r^S$)	critical points
1	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	1	3	sum of any 2 components of SVD
2	$\begin{pmatrix} 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	9	8	no interpretation
3	$\begin{pmatrix} 0 & 0 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	18	3	$\begin{pmatrix} 0 & 0 & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\operatorname{rank}(X_{\{2,3\},\{1,2\}}) = 1$
4	$\begin{pmatrix} 0 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	18	25	no interpretation
5*	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	36	3	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & 0 \\ 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & \cdot \\ 0 & \cdot & \cdot \end{pmatrix}$
6*	$\begin{pmatrix} 0 & 0 & \cdot \\ \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$	36	3	$\begin{pmatrix} 0 & 0 & 0 \\ \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\operatorname{rank}(X_{\{2,3\},\{1,2\}}) = 1$
7	$\begin{pmatrix} 0 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & 0 \end{pmatrix}$	6	30	no interpretation
8	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	9	1	projection onto $\mathcal{L}^S$
9*	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$	36	3	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \cdot & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ 0 & \cdot & \cdot \end{pmatrix}$
10*	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & \cdot \\ \cdot & \cdot & 0 \end{pmatrix}$	36	3	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \cdot & \cdot \\ \cdot & \cdot & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & \cdot \\ \cdot & \cdot & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & \cdot \\ 0 & \cdot & 0 \end{pmatrix}$
11*	$\begin{pmatrix} 0 & 0 & \cdot \\ \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \end{pmatrix}$	9	3	$\begin{pmatrix} 0 & 0 & 0 \\ \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \end{pmatrix}$ or $\operatorname{rank}(X_{\{2,3\},\{1,2\}}) = 1$
12*	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ \cdot & 0 & \cdot \end{pmatrix}$	36	3	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \cdot & 0 \\ \cdot & 0 & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & 0 \\ \cdot & 0 & \cdot \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ 0 & 0 & \cdot \end{pmatrix}$
13*	$\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ \cdot & 0 & 0 \end{pmatrix}$	6	3	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \cdot & 0 \\ \cdot & 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & 0 & 0 \\ \cdot & 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 & \cdot \\ 0 & \cdot & 0 \\ 0 & 0 & 0 \end{pmatrix}$

TABLE 8

The 13 orbit representatives of zero patterns of 3×3 matrices that have the property that there is no zero pattern S with less zeros such that the zero pattern of a critical point for S is contained in the orbit representative.

best rank-two approximation given by SVD has negative entries in S.

These facts lead to the following open questions.

QUESTION 6.3. 1. *Are the experimental observations (a) and (b) true for any nonnegative matrix $U \in \mathbb{R}^{3\times 3}$?*

2. *Given a nonnegative matrix $U \in \mathbb{R}^{m\times n}_{\geq 0}$ whose best nonnegative rank-2 approximation has zero pattern S, does the best rank-2 approximation given by SVD have negative entries in S?*
3. *For which zero patterns $S \subset [m] \times [n]$ and target ranks $r \in [m-1]$ there exists a full rank nonnegative matrix $U \in \mathbb{R}^{m\times n}_{\geq 0}$ whose best nonnegative rank-r approximation has zero pattern S?*

Acknowledgements. We thank Giorgio Ottaviani, Grégoire Sergeant-Perthuis, Pierre-Jean Spaenlehauer, and Bernd Sturmfels for helpful discussions and suggestions. Kaie Kubjas and Luca Sodomaco are partially supported by the Academy of Finland Grant No. 323416. Elias Tsigaridas is partially supported by ANR JCJC GALOP (ANR-17-CE40-0009), the PGMO grant ALMA, and the PHC GRAPE.

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