Counting Unique-Sink Orientations

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Abstract

Unique-sink orientations (USOs) are an abstract class of orientations of the n-cube graph. We consider some classes of USOs that are of interest in connection with the linear complementarity problem. We summarize old and show new lower and upper bounds on the sizes of some such classes. Furthermore, we provide a characterization of K-matrices in terms of their corresponding USOs.

Keywords: unique-sink orientation, linear complementarity problem, pivoting, P-matrix, K-matrix

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1 Introduction

Unique-sink orientations (USOs) are an abstract class of orientations of the n-cube graph. A number of concrete geometric optimization problems can be shown to have the combinatorial structure of a USO. Examples are the linear programming problem [11], and the problem of finding the smallest enclosing ball of a set of points [11, 30], or a set of balls [7]. In this paper, we count the USOs of the n-cube that are generated by P-matrix linear complementarity problems (P-USOs). This class covers many of the "geometric" USOs. We show that the number of P-USOs is $2^{\Theta(n^3)}$. The lower bound construction is the interesting contribution here, and it even yields USOs from the subclass of K-USOs, whose combinatorial structure is known to be very rigid [8]. In contrast, the number of all n-cube USOs is doubly exponential in n [17].

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Unique-sink orientations

We follow the notation of [8]. Let $[n] := \{1, 2, \ldots, n\}$. For a bit vector $v \in \{0,1\}^n$ and $I \subseteq [n]$, let $v \oplus I$ be the element of $\{0,1\}^n$ defined by

$$(v \oplus I)_j := \begin{cases} 1 - v_j & \text{if } j \in I, \\ v_j & \text{if } j \notin I. \end{cases}$$

Instead of $v \oplus \{i\}$ we write $v \oplus i$.

Under this notation, the (undirected) *n-cube* is the graph $G = (V, E)$ with

$$V := \{0,1\}^n, \quad E := \{\{v, v \oplus i\} : v \in V,\ i \in [n]\}.$$

A *subcube* of G is a subgraph $G' = (V', E')$ of G where $V' = \{v \oplus I : I \subseteq C\}$ for some vertex v and some set $C \subseteq [n]$, and $E' = E \cap \binom{V'}{2}$. The *dimension* of such a subcube is $|C|$.

Let ϕ be an orientation of the n-cube (a digraph with underlying undirected graph G). If ϕ contains the directed edge $(v, v \oplus i)$, we write $v \xrightarrow{\phi} v \oplus i$, or simply $v \to v \oplus i$ if ϕ is clear from the context. If V' is the vertex set of a subcube, then the directed subgraph of ϕ induced by V' is denoted by $\phi[V']$. For $F \subseteq [n]$, let $\phi^{(F)}$ be the orientation of the n-cube obtained by reversing all edges in coordinates contained in F; formally

$$v \xrightarrow{\phi^{(F)}} v \oplus i \quad :\Leftrightarrow \quad \begin{cases} v \xrightarrow{\phi} v \oplus i & \text{if } i \notin F, \\ v \oplus i \xrightarrow{\phi} v & \text{if } i \in F. \end{cases}$$

An orientation ϕ of the n-cube is a *unique-sink orientation* (*USO*) if every subcube $G' = (V', E')$ has a unique sink (that is, vertex of outdegree zero) in $\phi[V']$. It is not difficult to show that in a unique-sink orientation, every subcube also has a unique source (that is, vertex of indegree zero). More generally, if ϕ is a unique-sink orientation and $F \subseteq [n]$, then $\phi^{(F)}$ is a unique-sink orientation as well [30, Lemma 2.1].

A special USO is the *uniform orientation*, in which $v \to v \oplus i$ if and only if $v_i = 0$.

Unique-sink orientations enable a graph-theoretic description of simple principal pivoting algorithms for linear complementarity problems. They were introduced by Stickney and Watson [29] and have recently received much attention [10, 11, 12, 17, 21, 27, 28, 30].

Linear complementarity problems

A *linear complementarity problem* (LCP(M, q)) is for a given matrix $M \in \mathbb{R}^{n \times n}$ and a vector $q \in \mathbb{R}^n$, to find vectors $w, z \in \mathbb{R}^n$ such that

$$w - Mz = q, \quad w, z \geq 0, \quad w^T z = 0. \tag{1}$$

A *P-matrix* is a square real matrix whose principal minors are all positive. If M is a P-matrix, the appertaining LCP is called a *P-LCP*; in this case there exists a unique solution for any q [26].

Let $B \subseteq [n]$, and let A_B be the $n \times n$ matrix whose jth column is the jth column of $-M$ if $j \in B$, and the jth column of the $n \times n$ identity matrix I_n if $j \notin B$. If M is a P-matrix, then A_B is invertible for every set B. We call B a *basis*. If $A_B^{-1}q \geq 0$, let

$$w_i := \begin{cases} 0 & \text{if } i \in B \\ (A_B^{-1}q)_i & \text{if } i \notin B \end{cases}, \qquad z_i := \begin{cases} (A_B^{-1}q)_i & \text{if } i \in B \\ 0 & \text{if } i \notin B \end{cases}. \tag{2}$$

The vectors w, z are then a solution to the LCP (1).

A problem P-LCP(M, q) is *nondegenerate* if $(A_B^{-1}q)_i \neq 0$ for all B and i. Following [29], a nondegenerate P-LCP(M, q) induces a USO: For $v \in \{0,1\}^n$, let $B(v) := \{j \in [n] : v_j = 1\}$. Then the unique-sink orientation ϕ induced by P-LCP(M, q) is given by

$$v \xrightarrow{\phi} v \oplus i \quad :\Leftrightarrow \quad (A_{B(v)}^{-1}q)_i < 0. \tag{3}$$

The run of a simple principal pivoting method (see [23, Chapter 4]) for the P-LCP then corresponds to following a directed path in the orientation ϕ. Finding the sink of the orientation is equivalent to finding a basis B with $A_B^{-1}q \geq 0$, and thus via (2) to finding the solution to the P-LCP.

In this paper, we are primarily interested in establishing bounds for the number of n-dimensional USOs satisfying some additional properties (for instance, USOs induced by P-LCPs), which we introduce in the next section.

2 Matrix classes and USO classes

It is NP-complete to decide whether a solution to an LCP exists [2]. If the matrix M is a P-matrix, however, a solution always exists. The problem of finding it is unlikely to be NP-hard, because if it were, then NP = co-NP [18]. Even so, no polynomial-time algorithms for solving P-LCPs are known. Hence our motivation to study some special matrix classes and investigate what combinatorial properties their USOs have. The ultimate goal is then to try and exploit these combinatorial properties in order to find an efficient algorithm for the corresponding LCPs.

A *Z-matrix* is a square matrix whose off-diagonal entries are all non-positive. A *K-matrix* is a matrix which is both a Z-matrix and a P-matrix. A *hidden-K-matrix* is a P-matrix M such that there exist Z-matrices X and Y and non-negative vectors r and s with $MX = Y$, $r^T X + s^T Y > 0$. Taking X to be the identity matrix and $Y = M$, $s = 0$ and r any positive vector shows that every K-matrix is a hidden-K-matrix as well.

The importance of these matrix classes is due to the fact that polynomial-time algorithms are known for solving the LCP(M, q) if the matrix M is a Z-matrix [1, 25], a hidden-K-matrix [16], or the transpose of a hidden-K-matrix [24].

A USO is a *P-USO* if it is induced via (3) by some LCP(M, q) with a P-matrix M; it is a *K-USO* if it is induced by some LCP(M, q) with a K-matrix M; and it is a *hidden-K-USO* if it is induced by some LCP(M, q) with a hidden-K-matrix M.

A USO is a *Holt–Klee USO* if in each of its subcubes, there are d directed paths from the source to the sink of the subcube, with no two paths sharing a vertex other than source and sink; here d is the dimension of the subcube. A USO ϕ is *strongly Holt–Klee* if $\phi^{(F)}$ is Holt–Klee for every $F \subseteq [n]$. By [10], every P-USO is a strongly Holt–Klee USO.

Finally, a USO is *locally uniform*, if

$$\begin{aligned} &\text{whenever } v_i = v_j = 0 \text{ and } v \xrightarrow{\phi} v \oplus i,\ v \xrightarrow{\phi} v \oplus j, \\ &\qquad\qquad\text{then } v \oplus i \xrightarrow{\phi} v \oplus \{i,j\},\ v \oplus j \xrightarrow{\phi} v \oplus \{i,j\} \end{aligned} \tag{4}$$

and

$$\begin{aligned} &\text{whenever } v_i = v_j = 0 \text{ and } v \oplus i \xrightarrow{\phi} v,\ v \oplus j \xrightarrow{\phi} v, \\ &\qquad\qquad\text{then } v \oplus \{i,j\} \xrightarrow{\phi} v \oplus i,\ v \oplus \{i,j\} \xrightarrow{\phi} v \oplus j. \end{aligned} \tag{5}$$

By [8], every K-USO is locally uniform, and every locally uniform USO is acyclic. We thus have the following chain of inclusions, some of which are in fact strict:

$$\begin{aligned} &\text{K-USOs} \subseteq \text{locally uniform P-USOs} \subset \text{acyclic P-USOs} \subset \text{P-USOs} \\ &\qquad\qquad \subset \text{strongly Holt–Klee USOs} \subset \text{Holt–Klee USOs}. \end{aligned}$$

The first inclusion is not known to be strict; see also Section 4. The second inclusion is easily seen to be strict already for $n = 2$. Strictness of the third inclusion is due to Stickney and Watson: there exists a cyclic P-USO of the 3-cube [29]. The fourth inclusion is strict as a consequence of our counting results: the number of strongly Holt–Klee USOs is much larger than the number of P-USOs. Finally, there is an example that shows strictness of the fifth inclusion [10, Fig. 12].

An *LP-USO* is an orientation of the n-cube admitting a realization $r : \{0,1\}^n \to \mathbb{R}^n$ as a polytope in the n-dimensional Euclidean space, combinatorially equivalent to the n-cube, such that there exists a linear function $f : \mathbb{R}^n \to \mathbb{R}$ and

$$v \xrightarrow{\phi} v \oplus i \quad \text{if and only if} \quad f(r(v \oplus i)) > f(r(v)).$$

It follows from [13, 14, 20, 22, 24] that LP-USOs are exactly hidden-K-USOs, and we have:

$$\text{K-USOs} \subset \text{LP-USOs} = \text{hidden-K-USOs} \subseteq \text{acyclic P-USOs}.$$

Again, the first inclusion is strict already for $n = 2$; it is open whether the last inclusion is strict. In the next section we examine the numbers of n-USOs in the respective classes.

It is also possible to obtain USOs from completely general linear programs. The reduction in [11] yields *PD-USOs*, i.e., USOs generated by LCPs with symmetric positive definite matrices M. Since these are exactly the symmetric P-matrices [3, Section 3.3], we also have PD-USOs $\subseteq$ P-USOs, where we do not know whether the inclusion is strict. The USOs that are obtained from the problem of finding the smallest enclosing ball of a set of points [9, Section 3.2] are "almost" PD-USOs in the sense that every subcube not containing the origin 0 is oriented by a PD-USO [19]. For the USOs from smallest enclosing balls of *balls* [7], we are not aware of a similar result.

3 Counting USOs

In this section, we examine the number of USOs in the classes described above, depending on their dimension. The n-cube as we have introduced it is a labelled graph; accordingly, the counting will be in the labelled sense. But all the bounds are valid also for the number of isomorphism classes of USOs: the n-cube has $2^n n! = 2^{\Theta(n \log n)}$ automorphisms, so the labelled and unlabelled counts differ by at most this factor—which is negligible, since all our bounds are at least of the order $2^{\Omega(n^3)}$.

First counting results about USOs were obtained by Matoušek [17], who gave asymptotic bounds on the number of all USOs and acyclic USOs.

Next, Develin [5]—in order to show that the Holt–Klee condition does not characterize LP-USOs—proved that the number of n-dimensional LP-USOs is bounded from above by $2^{O(n^3)}$, whereas the number of Holt–Klee USOs is bounded from below by $2^{\Omega(2^n/\sqrt{n})}$.

Using similar means, we prove an upper bound of $2^{O(n^3)}$ on the number of P-USOs, and observe that a slight modification of Develin's construction yields a lower bound of $2^{\binom{n-1}{\lfloor (n-1)/2 \rfloor}} = 2^{\Omega(2^n/\sqrt{n})}$ for strongly Holt–Klee locally uniform USOs. Furthermore, we provide a construction of $2^{\Omega(n^3)}$ K-USOs. These results imply that the number of K-USOs, LP-USOs, as well as P-USOs, is $2^{\Theta(n^3)}$.

Previously known and new bounds on the number of n-dimensional USOs in the classes defined in the previous section are summarized in the following table. Where an entry is missing, the best known bound coincides with the one of a subclass or a superclass; see also Section 2. We note that already before Develin's counting result [5], it had been shown by Morris [20] that the Holt–Klee condition does not characterize P-USOs, starting from dimension $n = 4$.

class	lower bound	upper bound
K-USOs	$2^{\Omega(n^3)}$	
LP-USOs		$2^{O(n^3)}$ [5]
P-USOs		$2^{O(n^3)}$
acyclic strongly Holt–Klee USOs	$2^{\Omega(2^n/\sqrt{n})}$	
Holt–Klee USOs	$2^{\Omega(2^n/\sqrt{n})}$ [5]	
locally uniform USOs	$2^{\Omega(2^n/\sqrt{n})}$	
acyclic USOs [17]	$2^{2^{n-1}}$	$(n+1)^{2^n}$
all USOs [17]	$n^{\Omega(2^n)}$	$n^{O(2^n)}$

3.1 An upper bound for P-USOs

Every P-USO is determined by the sequence $\sigma(M,q) = \big(\mathrm{sgn}(A_{B(v)}^{-1}q)_i : v \in \{0,1\}^n,\ i \in [n]\big)$, which is a function of the P-matrix M and the right-hand side q. Furthermore, we are interested only in nondegenerate right-hand sides q, which means we are interested only in sequences containing no 0.

3.1 Lemma. *Each entry of the vector $\sigma(M,q)$ is the sign of a polynomial in the entries of M and q of degree at most n.*

Proof. The entries of the matrix $A_{B(v)}^{-1}$ can be computed as

$$(A_{B(v)}^{-1})_{rs} = \frac{1}{\det A_{B(v)}}(-1)^{r+s}A_{sr},$$

where A_{ij} is the determinant of the submatrix of $A_{B(v)}$ obtained by deleting the ith row and the jth column, which is a polynomial of degree at most $n-1$. Hence

$$(A_{B(v)}^{-1}q)_i = \frac{1}{\det A_{B(v)}}\sum_{s=1}^{n} q_s \cdot (-1)^{i+s} \cdot A_{si}.$$

Recall that $A_{B(v)}$ has $|B(v)|$ columns of $-M$ and $n-|B(v)|$ columns of the identity matrix; thus $\operatorname{sgn}\det A_{B(v)} = (-1)^{|B(v)|}$, since M is a P-matrix. Therefore

$$\operatorname{sgn}(A_{B(v)}^{-1}q)_i = \operatorname{sgn}\Big((-1)^{|B(v)|} \cdot \sum_{s=1}^{n} q_s \cdot (-1)^{i+s} \cdot A_{si}\Big),$$

which is the sign of a polynomial of degree at most n. ☐

The algebraic tool we will apply is the following theorem.

3.2 Theorem (Warren [31])**.** *Let $p_1, \dots, p_\ell$ be real polynomials in k variables, each of degree at most d. For $\ell \geq k$, the number of sign sequences $\sigma(x) = (\operatorname{sgn} p_1(x), \dots, \operatorname{sgn} p_\ell(x))$ that consist of terms $+1$, -1 is at most $(4ed\ell/k)^k$.*

Now all is set to prove an upper bound on the number of P-USOs.

3.3 Theorem. *The number of distinct n-dimensional P-USOs is at most $2^{O(n^3)}$.*

Proof. By Lemma 3.1, each P-USO is determined by a vector of $\ell = n2^n$ nonzero signs of polynomials of degree at most n. The number of variables is $k = n^2 + n$ (equal to the number of entries of the matrix M and the vector q). By Theorem 3.2, there are at most

$$\left(\frac{4e \cdot n \cdot n2^n}{n^2+n}\right)^{n^2+n} \leq (4e \cdot 2^n)^{n^2+n} = 2^{O(n^3)}$$

such sign vectors. ☐

3.2 A lower bound for strongly Holt–Klee and locally uniform USOs

Recall that a *strongly Holt–Klee orientation* is a Holt–Klee orientation ϕ that remains so after flipping all the edges in any given subset of coordinates, that is, if $\phi^{(F)}$ is Holt–Klee for any $F \subseteq [n]$.

A *monotone Boolean function* is a function $f : \{0,1\}^k \to \{0,1\}$ such that if $x \leq y$, then $f(x) \leq f(y)$; in "$x \leq y$", $\leq$ is to be understood component-wise. Counting monotone Boolean functions is known as *Dedekind's problem* [4]. Let M be the set of $0,1$-vectors of length k with exactly $\lfloor k/2 \rfloor$ ones. Following [15], a lower bound of $2^{\binom{k}{\lfloor k/2 \rfloor}}$ on the number of k-variate monotone Boolean functions can be obtained by taking for each subset $A \subseteq M$ the function f_A given by

$$f_A(x) = 1 \quad \text{iff} \quad \{y \in A : y \leq x\} \neq \emptyset.$$

This means, f_A attains value 1 exactly on the 0,1-vectors in A and all the ones that are larger (w.r.t. the order $\leq$).

3.4 Theorem. *The number of acyclic locally uniform strongly Holt–Klee n-USOs is at least* $2^{\binom{n-1}{\lfloor (n-1)/2 \rfloor}} = 2^{\Omega(2^n/\sqrt{n})}$.

Proof. Given an $(n-1)$-variate monotone Boolean function f, we construct an n-USO ϕ by setting

$$v \xrightarrow{\phi} v \oplus i \text{ if } i \neq n \text{ and } v_i = 0,$$
$$v \xrightarrow{\phi} v \oplus n \text{ if } v_n + f(v') = 1,$$

where $v' \in \{0,1\}^{n-1}$ is formed by the initial $n-1$ bits of v, and addition in the second equation is modulo 2. It is easy to see that this indeed defines a USO: on both facets $\{v : v_n = 0\}$ and $\{v : v_n = 1\}$, we have the same (uniform) orientation, and this is already sufficient to guarantee the USO properties. Between the two facets, we have $(v', 0) \xrightarrow{\phi} (v', 1)$ if and only if $f(v') = 1$.

The USO ϕ is clearly acyclic because any directed walk in ϕ is monotone on the first $n-1$ bits. It is easy to show local uniformity too. The assumption of (5) is never satisfied. For (4) it suffices to consider the case $j = n$: If $v \xrightarrow{\phi} v \oplus n$, then $f(v') = 1$, thus by monotonicity $f((v \oplus i)') = 1$. Hence $v \oplus i \xrightarrow{\phi} v \oplus \{i, n\}$.

For the strong Holt–Klee property, let $F \subseteq [n]$ and let $V' = \{v \oplus I : I \subseteq C\}$ be the vertex set of a subcube with $|C| =: d$. If $n \notin C$, then $\phi^{(F)}[V']$ is isomorphic to the uniform orientation, which is easily seen to satisfy the Holt–Klee property. So suppose $n \in C$. Let $V_0 := \{v \in V' : v_n = 0\}$ and $V_1 := \{v \in V' : v_n = 1\}$ and let s be the source and t the sink of $\phi^{(F)}[V']$. Note that $\phi^{(F)}[V_0]$ and $\phi^{(F)}[V_1]$ are identical if we truncate the last coordinate of their vertices, and isomorphic to the uniform USO.

Now we distinguish two cases. First, if both s and t lie in the same set V_0 or V_1, that is, if $b := s_n = t_n$, then there are $d-1$ disjoint paths from s to t in $\phi^{(F)}[V_b]$ and another path obtained by concatenating the edge $s \to s \oplus n$, a path in $\phi^{(F)}[V_{1-b}]$ from $s \oplus n$ to $t \oplus n$, and the edge $t \oplus n \to t$.

Second, let $b := s_n = 1 - t_n$. Without loss of generality we may assume that $b = 0$ and $n \notin F$. Let $P(i_1, \ldots, i_d)$ denote the directed path $s \to s \oplus \{i_1\} \to s \oplus \{i_1, i_2\} \to \cdots \to s \oplus \{i_1, i_2, \ldots, i_d\}$. Order the elements of $C \setminus \{n\} = \{j_1, j_2, \ldots, j_{d-1}\}$ so that for $j_k \in F$ and $j_\ell \notin F$ we have $k < \ell$. Since $\phi^{(F)}[V_0]$ and $\phi^{(F)}[V_1]$ are both isomorphic to the uniform orientation and $s_n \neq t_n$, we have $t = s \oplus C$. Now we claim that the paths $P(j_1, j_2, \ldots, j_{d-1}, n)$, $P(j_2, j_3, \ldots, j_{d-1}, n, j_1)$, $\ldots$, $P(j_{d-1}, n, j_1, j_2, \ldots, j_{d-2})$, $P(n, j_1, j_2, \ldots, j_{d-1})$ are vertex-disjoint directed paths from s to t. The only non-obvious fact to show is that for any $k \in [d]$, there is a directed edge $u := s \oplus \{j_k, j_{k+1}, \ldots, j_{d-1}\} \to$

$v := s \oplus \{j_k, j_{k+1}, \ldots, j_{d-1}, n\}$. Note that $u \to v$ if and only if $f(u') = 1$ and that $f(s') = f(t') = 1$. If $j_k \notin F$, then $s' \leq u'$ and so $1 = f(s') \leq f(u')$, thus $f(u') = 1$. If on the other hand $j_k \in F$, then $t' \leq u'$ and so $1 = f(t') \leq f(u')$, thus $f(u') = 1$. Hence $u \to v$.

Therefore the number of acyclic locally uniform strongly Holt–Klee n-USOs is lower bounded by the number of $(n-1)$-variate monotone Boolean functions, which concludes the proof. □

Remark. After swapping the roles of 0 and 1 in the nth coordinate, the above construction is the same as Mike Develin's construction [5] of many orientations satisfying the Holt–Klee condition. Thus, both Develin's and our construction yield Holt–Klee orientations, but local uniformity is obtained only in our variant.

The logarithm of the total number of acyclic n-USOs is no more than $2^n \log(n+1)$ [17]. In comparison, the exponent in the lower bound obtained from Theorem 3.4 is of the order $2^n/\sqrt{n}$, and therefore still exponential. Restricting to K-USOs, the exponent goes down to a polynomial in n.

3.3 A lower bound for K-USOs

3.5 Theorem. *The number of distinct K-USOs in dimension n is at least $2^{\Omega(n^3)}$.*

Proof. Consider the upper triangular matrix

$$M(\beta) = \begin{pmatrix} 1 & -1-\beta_{1,2} & -1-\beta_{1,3} & \ldots & -1-\beta_{1,n} \\ 0 & 1 & -1-\beta_{2,3} & \ldots & -1-\beta_{2,n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \ldots & -1-\beta_{n-1,n} \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}$$

and the vector $q = (-1, 1, -1, \ldots, (-1)^n)^T$. If the parameters $\beta_{i,j}$ are sufficiently small in absolute value, then $M(\beta)$ is a K-matrix. We will now examine how the choice of the $\beta_{i,j}$ influences the USO induced by the LCP$(M(\beta), q)$. Our goal is to show that we can make $2^{\Omega(n^3)}$ choices, each of which induces a different USO.

From now on, we will write

$$(i,j) \prec (i',j') \quad \text{for} \quad (j < j') \text{ or } (j = j' \text{ and } i > i').$$

Note that $\prec$ is a total ordering on $\{(i,j) \in [n]^2 : i < j\}$. The strategy will be to choose the values of the $\beta_{i,j}$ in the order given by $\prec$, that is, from left to right and in each column from bottom to top. We show that for about half of the $\beta_{i,j}$'s there is a number of choices exponential in $j - i$ such that each of these choices determines a different orientation on a certain subset of edges, which will be independent of all subsequently made choices. But first we examine the expressions that determine the orientation.

Let $B \subseteq [n]$ and, analogously to the definition of A_B, let $A_B(\beta)$ be the matrix whose jth column is the jth column of $-M(\beta)$ if $j \in B$, and the jth column of I_n otherwise.

3.6 Lemma. *The entries of the inverse matrix* $(A_B(\beta))^{-1}$ *of* $A_B(\beta)$ *satisfy*

$$\sigma_r \cdot \left((A_B(\beta))^{-1}\right)_{r,s} = \begin{cases} 1 & \text{if } r = s, \\ 0 & \text{if } r > s \text{ or if } r < s \text{ and } s \notin B, \\ 2^{p(B,r,s)} + \beta_{r,s} + t_{B,r,s}(\beta) & \text{if } r < s \text{ and } s \in B, \end{cases} \tag{6}$$

where $\sigma_r = -1$ *if* $r \in B$ *and* $\sigma_r = 1$ *if* $r \notin B$, $p(B, r, s) = |\{j \in B : r < j < s\}|$ *and* $t_{B,r,s}(\beta)$ *is a polynomial with positive coefficients and no constant term, in exactly the variables* $\beta_{i,j}$ *for*

$$(i, j) \in J_{r,s}(B) := \{(i, j) \in (B \cup \{r\}) \times B : r \leq i < j, (i, j) \prec (r, s)\}. \tag{7}$$

Proof. The inverse of an upper triangular matrix is again upper triangular. Its diagonal entries are the reciprocals of the diagonal entries of the original matrix; in our case, they are ± 1. Moreover, for $s \notin B$, the sth column of $(A_B(\beta))^{-1}$ equals the sth unit vector e_s, the unique solution of the equation system $A_B(\beta)x = e_s$.

So it remains to examine the above-diagonal entries in columns belonging to B. Such entries only exist if $B\backslash\{1\} \neq \emptyset$, and they are indexed by $J(B) = \{(r, s) \in [n] \times B : r < s\}$. Consider the ordering $\prec$ defined above, restricted to $J(B)$. The least element of $J(B)$ with respect to $\prec$ is $(s - 1, s)$, where s is the least element of $B \setminus \{1\}$. Multiplying row $s - 1$ of $A_B(\beta)$ with the sth column of $(A_B(\beta))^{-1}$ reveals that $\left((A_B(\beta))^{-1}\right)_{s-1,s} = \sigma_{s-1} \cdot (1 + \beta_{s-1,s})$. Thus (6) holds for the $\prec$-minimum (r, s) in $J(B)$.

For any other $(r, s) \in J(B)$, assume that (6) holds for all $(k, s) \prec (r, s)$. Multiplying the rth row of $A_B(\beta)$ by the sth column of $(A_B(\beta))^{-1}$ shows that

$$\underbrace{\sigma_r}_{A_B(\beta)r,r} \cdot \left((A_B(\beta))^{-1}\right)_{r,s} + \sum_{\substack{k \in B \\ r<k<s}} \underbrace{(1 + \beta_{r,k})}_{A_B(\beta)_{r,k}} \cdot \underbrace{\sigma_k \cdot \left(2^{p(B,k,s)} + \beta_{k,s} + t_{B,k,s}(\beta)\right)}_{((A_B(\beta))^{-1})_{k,s}}$$
$$+ \underbrace{(1 + \beta_{r,s})}_{A_B(\beta)_{r,s}} \cdot \underbrace{\sigma_s}_{((A_B(\beta))^{-1})_{s,s}} = 0.$$

As $\sigma_k = \sigma_s = -1$ for $k, s \in B$, we have

$$\begin{aligned} \sigma_r \cdot \left((A_B(\beta))^{-1}\right)_{r,s} &= \beta_{r,s} + 1 + \sum_{\substack{k \in B \\ r<k<s}} (1 + \beta_{r,k}) \left(2^{p(B,k,s)} + \beta_{k,s} + t_{B,k,s}(\beta)\right) \\ &= \beta_{r,s} + 1 + \sum_{\substack{k \in B \\ r<k<s}} 2^{p(B,k,s)} + t_{B,r,s}(\beta) \\ &= \beta_{r,s} + 2^{p(B,r,s)} + t_{B,r,s}(\beta), \end{aligned} \tag{8}$$

where

$$t_{B,r,s}(\beta) := \sum_{\substack{k \in B \\ r<k<s}} \left(2^{p(B,k,s)}\beta_{r,k} + \beta_{k,s} + \beta_{r,k}\beta_{k,s} + t_{B,k,s}(\beta) + \beta_{r,k}t_{B,k,s}(\beta)\right) \tag{9}$$

is a polynomial with positive coefficients and no constant term, as required. The variables appearing in this polynomial are indexed by the set

$$\bigcup_{\substack{k \in B \\ r<k<s}} \big(\{(r,k),(k,s)\} \cup J_{k,s}(B)\big) = J_{r,s}(B). \qquad \square$$

We next investigate the vectors $(A_B(\beta))^{-1}q$ whose sign patterns determine the orientations of the edges in the unique sink orientation; see (3). First we identify a large number of bases B for which the signs in $(A_B(\beta))^{-1}q$ are sensitive to very small changes in β.

Let $B \subseteq [n]$ be a basis such that, for $m = \max B$, we have $s \equiv m+1 \pmod 2$ for each $s \in B \setminus \{m\}$. Then $q_m \cdot q_s = -1$ for each $s \in B \setminus \{m\}$, and hence for all $r < m$ such that $r \equiv m+1 \pmod 2$,

$$\begin{aligned}\sigma_r \cdot \big((A_B(\beta))^{-1}q\big)_r &= (-1)^m \Bigg(\beta_{r,m} + t_{B,r,m}(\beta) - \sum_{\substack{s \in B \\ r<s<m}} \big(\beta_{r,s} + t_{B,r,s}(\beta)\big)\Bigg) \\ &= (-1)^m \big(\beta_{r,m} - t'_{B,r,m}(\beta)\big); \qquad (10)\end{aligned}$$

the parity condition on r and m ensures that the constant terms sum to zero. Each $t'_{B,r,m}(\beta)$ is some polynomial in variables $\beta_{i,j}$ for $(i,j) \in \{(i,j) \in [n] \times B : i<j,\ (i,j) \prec (r,m)\}$ with no constant term. In particular, this implies that in the corresponding USO, the orientation of the rth edge incident to the vertex corresponding to the basis B depends only on the values of $\beta_{i,j}$ with $(i,j) \preceq (r,m)$.

Now let $r, m \in [n]$, $r < m$, $r \equiv m+1 \pmod 2$. Let

$$C = C(r,m) = \{i \in [n] : r < i < m,\ i \equiv m+1 \,(\mathrm{mod}\ 2)\}$$

and let

$$V' = V'(r,m) = \{(0 \oplus m) \oplus I : I \subseteq C\}.$$

Note that $|C| = (m-r-1)/2$ and so $|V'| = 2^{(m-r-1)/2}$.

Furthermore, suppose for a moment that the values of $\beta_{i,j}$ are fixed for all $(i,j) \prec (r,m)$, and that these values satisfy:

$$v, v' \in V',\ v \neq v' \quad \Longrightarrow \quad t'_{B(v),r,m}(\beta) \neq t'_{B(v'),r,m}(\beta). \qquad (11)$$

For each $v \in V'$, the direction of the edge between v and $v \oplus r$ in the USO induced by $\mathrm{LCP}(M(\beta), q)$ is by (10) determined by the sign of the difference $\beta_{r,m} - t'_{B(v),r,m}(\beta)$. By (11), the currently fixed values of $t'_{B(v),r,m}$ for $v \in V'$ are all distinct and thus they split the reals into $|V'|+1$ intervals. Hence there are $|V'|+1$ choices for $\beta_{r,m}$ so that the resulting USOs will differ from one another in the orientation of at least one of these edges.

What happens, though, if we are about to choose $\beta_{r,m}$ and (11) is not satisfied? Then we have to revise the choices we have made so far. Slightly perturbing each $\beta_{i,j}$ with $(i,j) \prec (r,m)$ will not change the orientation (because each $\beta_{i,j}$ is chosen in the *interior* of one of the $|V'|+1$ intervals mentioned above); the next lemma implies that it will make (11) satisfied.

3.7 Lemma. *Let $r, m \in [n]$, $r < m$, $r \equiv m+1 \pmod 2$ and let $B_1, B_2 \subseteq [n]$ be bases such that $\max B_1 = \max B_2 = m$, $\min B_1 > r$, $\min B_2 > r$, and that $i \equiv m+1 \pmod 2$ for all $i \in (B_1 \cup B_2) \setminus \{m\}$. Then the polynomial $t'_{B_1,r,m}(\beta) - t'_{B_2,r,m}(\beta)$ is identically zero if and only if $B_1 = B_2$.*

Proof. First, from (10) we have:

$$t'_{B,r,m}(\beta) = -t_{B,r,m}(\beta) + \sum_{\substack{s \in B \\ r<s<m}} \bigl(\beta_{r,s} + t_{B,r,s}(\beta)\bigr). \tag{12}$$

Assume that $B_1 \neq B_2$. Without loss of generality, there exists some $u \in B_1 \setminus B_2$; by assumption $u > r$. It follows from (12) and the properties of the polynomials t guaranteed by Lemma 3.6 that $t'_{B_1,r,m}(\beta)$ contains the variable $\beta_{u,m}$ while $t'_{B_2,r,m}(\beta)$ does not. Hence $t'_{B,r,m}(\beta) - t'_{B',r,m}(\beta)$ is not identically zero. The converse implication is trivial. $\square$

The options to choose $\beta_{r,m}$ are, of course, not independent of the values of the other $\beta_{i,j}$'s. However, they depend only on the $\beta_{i,j}$'s with $(i,j) \prec (r,m)$. Hence it is possible to make the choices sequentially in the order given by $\prec$; starting with $\beta_{1,2}$ and finishing with $\beta_{1,n}$. The values of $\beta_{r,m}$ for $r \equiv m \pmod 2$ can be chosen arbitrarily, e.g., $\beta_{r,m} = 0$.

Therefore the number of distinct USOs induced by $\mathrm{LCP}(M(\beta), q)$ for various values of $\beta_{i,j}$, as described above, is at least

$$\prod_{m=1}^{n} \prod_{\substack{1 \le r < m \\ r \equiv m+1 \,(\mathrm{mod}\ 2)}} \Bigl(2^{(m-r-1)/2} + 1\Bigr) = \prod_{m=1}^{n} \prod_{i=0}^{\lfloor m/2 \rfloor - 1} \bigl(2^i + 1\bigr) = 2^{\Omega(n^3)}. \tag{13}$$

Finally, it remains to show that the values of all $\beta_{i,j}$'s can be chosen to satisfy $|\beta_{i,j}| < 1$, so that $M(\beta)$ would be a K-matrix. That follows from the next lemma.

3.8 Lemma. *Whenever $t'_{B,r,m}$ as in (12) is defined, let*

$$\bar\beta = \max\bigl\{|\beta_{i,j}| : (i,j) \in [n] \times B,\ i < j,\ (i,j) \prec (r,m)\bigr\}.$$

If $\bar\beta < 1$, then $|t'_{B,r,m}(\beta)| < 4^{m-r+1}\bar\beta$.

Proof. By definition, $p(B,j,s) \le s-j-1$ for all eligible B, j, s. Now we claim that

$$|t_{B,r,s}(\beta)| \le 4^{s-r}\bar\beta, \tag{14}$$

with $t_{B,r,s}(\beta)$ as in (9). If $s-r=1$ or $\bar\beta = 0$, then by (9) we have $t_{B,r,s}(\beta) = 0 \le 4^{s-r}\bar\beta$. Otherwise, by induction on $s-r$, again using (9) and $\bar\beta^2 < \bar\beta < 1$, we have

$$\begin{aligned}
|t_{B,r,s}(\beta)| &\le \sum_{j=r+1}^{s-1} \Bigl(2^{p(B,j,s)}\bar\beta + \bar\beta + \bar\beta^2 + 4^{s-j}\bar\beta + 4^{s-j}\bar\beta^2\Bigr) \\
&\le \sum_{j=r+1}^{s-1} \bigl(2^{s-j-1} + 2 + 2\cdot 4^{s-j}\bigr)\,\bar\beta \le \sum_{j=r+1}^{s} \bigl(3\cdot 4^{s-j}\bigr)\,\bar\beta = (4^{s-r}-1)\bar\beta \le 4^{s-r}\bar\beta.
\end{aligned}$$

Thus (14) holds.

Finally, unless $\bar{\beta} = 0$, in which case $t'_{B,r,s}(\beta) = 0$, we conclude from (12) and (14) that

$$
\begin{aligned}
|t'_{B,r,m}(\beta)| &\leq \left(4^{m-r} + (m-r-1) + \sum_{s=r+1}^{m-1} 4^{s-r}\right)\bar{\beta} \\
&= \left(m - r - 1 + \tfrac{1}{3}(4^{m-r+1} - 4)\right)\bar{\beta} \\
&\leq 4^{m-r+1}\bar{\beta}. \qquad \square
\end{aligned}
$$

The first β to be chosen is $\beta_{1,2}$, and its sign determines the direction of the edge between $(0, 1, 0, \ldots, 0)$ and $(1, 1, 0, \ldots, 0)$. If $\beta_{1,2}$ is chosen to be $\pm(4 + \epsilon)^{-n^3}$, then all subsequent choices can be made in such a way that $|\beta_{r,s}| < 1$ for all r, s. $\square$

3.4 The number of USOs from a fixed matrix

In this section, we prove the following

3.9 Theorem. *For a P-matrix $M \in \mathbb{R}^{n \times n}$, let $u(M)$ be the number of USOs determined by LCPs of the form* $\mathrm{LCP}(M, q)$ *for $q \in \mathbb{R}^n$. Furthermore, define $u(n) = \max_M u(M)$, where the maximum is over all $n \times n$ P-matrices. Then*

$$u(n) = 2^{\Theta(n^2)}.$$

Proof. Let us first show the upper bound. For a fixed M, we consider the $n2^n$ hyperplanes of the form

$$\left\{x \in \mathbb{R}^n : (A_{B(v)}^{-1} x)_i = 0\right\}.$$

These hyperplanes determine an *arrangement* that subdivides $\mathbb{R}^n$ into faces of various dimensions. Each face is an inclusion-maximal region over which the sign vector $\left(\mathrm{sgn}(A_{B(v)}^{-1} x)_i : v \in \{0,1\}^n, i \in [n]\right)$ is constant. The faces of dimension n are called *cells*; within a cell, the sign vector is nonzero everywhere. From Section 3.1 we know that $\mathrm{LCP}(M, q)$ yields a USO whenever q is in some cell, and for all q within the same cell, $\mathrm{LCP}(M, q)$ yields the same USO. Thus, the number of cells in the arrangement is an upper bound for the number $u(M)$ of different USOs induced by M. It is well-known [6] that the number of cells in an arrangement of N hyperplanes in dimension n is $O(N^n)$. In our case, we have $N = n2^n$ which shows that $u(M) = O((n2^n)^n) = 2^{O(n^2)}$ for all M.

For the lower bound, note that we have in particular constructed in Section 3.3 a K-matrix $M' \in \mathbb{R}^{(n-1)\times(n-1)}$ (resulting from fixing $\beta_{i,j}$ for all $j < n$), with the following property: for a suitable right-hand side q, $\mathrm{LCP}(M, q)$ with

$$M = \begin{pmatrix} M' & b \\ 0 & 1 \end{pmatrix}$$

yields $2^{\Omega(n^2)}$ different USOs in the subcube F corresponding to vertices with $v_n = 1$, when b is varied. This number is the term for $m = n$ in (13).

Since the subcube F corresponds to the solutions of $w - Mz = q$ that satisfy $w_n = 0$, we have $z_n = q_n$ within F. With $w' = (w_1, \dots, w_{n-1})^T$, $z' = (z_1, \dots, z_{n-1})^T$ and $q' = (q_1, \dots, q_{n-1})^T$, it follows that

$$w - Mz = q, \quad w^T z = 0, \quad w_n = 0$$

if and only if

$$w' - M'z' = q' + bq_n, \quad w'^T z' = 0, \quad z_n = q_n.$$

This is easily seen to imply that the induced USO in the subcube F is generated by $\mathrm{LCP}(M', q' + bq_n)$. Thus, $u(M') = 2^{\Omega(n^2)}$, and the theorem is proved. □

4 Locally uniform USOs and K-matrices

Finally we present a note on the relationship between K-matrices and locally uniform USOs.

4.1 Theorem. *Let M be a P-matrix. M is a K-matrix if and only if for all nondegenerate q, the USO induced by* $\mathrm{LCP}(M, q)$ *is locally uniform.*

Proof. The "only-if" direction is Proposition 5.3 in [8]. For the if-direction, suppose that M is not a K-matrix. We will construct a vector q such that the induced USO violates (4). First, since M is not a K-matrix, there exists an off-diagonal entry $m_{ij} > 0$, $i \neq j$. W.l.o.g. assume that $\{i, j\} = \{1, 2\}$ and define

$$Q = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}.$$

Let us now consider $B = \{1, 2\}$. Then

$$A_B = \left(\begin{array}{c|c} -Q & 0 \\ \hline 0 & I_{n-2} \end{array}\right),$$

and

$$A_B^{-1} = \left(\begin{array}{c|c} -Q^{-1} & 0 \\ \hline 0 & I_{n-2} \end{array}\right),$$

where

$$-Q^{-1} = \frac{1}{\det(Q)} \begin{pmatrix} -m_{22} & m_{12} \\ m_{21} & -m_{11} \end{pmatrix} = \frac{1}{m_{11}m_{22} - m_{21}m_{12}} \begin{pmatrix} -m_{22} & m_{12} \\ m_{21} & -m_{11} \end{pmatrix}.$$

Since Q is a P-matrix, its determinant is positive, hence $-Q^{-1}$ has some positive off-diagonal entry. Suppose first that $m_{12} > 0$. Then we set $q = (-m_{12}, -(m_{22}+1), 0, \dots, 0)$ and observe that

$$(A_B^{-1} q)_1 = \frac{-m_{12}}{m_{11}m_{22} - m_{21}m_{12}} < 0.$$

Slightly perturbing q such that it becomes nondegenerate will not change this strict inequality. But this is a contradiction to (4): at $B = \emptyset$, the edges in directions 1 and 2 are outgoing due to $q_1, q_2 < 0$ (note that $m_{22} > 0$ because M is a P-matrix), but at $B = \{1, 2\}$, the edge in direction 1 is *not* incoming as required by (4). If $m_{21} > 0$, the vector $q = (-(m_{11} + 1), -m_{21}, 0, \ldots, 0)$ leads to the same contradiction. $\square$

Remark. It may be more interesting to answer the following open question: Is it true that every locally uniform P-USO is a K-USO?

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