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NEW UPPER BOUNDS ON THE PROBABILITY OF EVENTS BASED ON GRAPH STRUCTURES

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(*communicated by A. Prékopa*)

Abstract. We present upper bounds for the probability of the union of events based on the individual probabilities and joint probabilities of pairs. The bounds generalize Hunter's upper bound and can be interpreted as objective function values corresponding to feasible solutions of the dual of the Boolean probability bounding LP.

1. Introduction

The problem to compute lower and upper bounds for the probability of the union of events has been mentioned already in the works of Boole [2]-[4]. Important further results to the topic was obtained by Bonferroni [1]. The topic has many applications in probability theory, statistics, reliability theory, and stochastic programming. Therefore intensive research efforts have been made in this field even recently [5]-[6], [8]-[21].

One of the important upper bounds is due to Hunter [10]. It is based on a special graph structure called spanning tree. The aim of this paper is to find upper bounds using different graphs.

Section 2 describes the linear programming problem to compute or approximate the probability of events discovered by Boole. The new bounds are provided in Section 3.

2. The Boolean probability bounding LP

In this section we summarize some of the results that we make use in the present paper. The Boolean probability bounding LP (see [9], [15], [16]) can be formulated in the following way.

Let $A_1, \ldots, A_n$ be events. Let $\mathcal{N} = \{1, \ldots, n\}$ be the set of indices. For any subset $\mathcal{J} \subseteq \mathcal{N}$ its complement is denoted by $\bar{\mathcal{J}}$. Let

$$\emptyset \neq \mathcal{I} \subseteq 2^{\mathcal{N}}$$

be an arbitrary set. Assume that the probabilities

$$p_{\mathcal{J}} = P(\cap_{i \in \mathcal{J}} A_i)$$

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are known for each element $\mathcal{J}$ of $\mathcal{I}$. Let $\mathcal{L} \subseteq \mathcal{N}$ be an arbitrary subset. Let $x_{\mathcal{L}}$ be the probability that exactly the events in $\mathcal{L}$ occur, i.e.

$$x_{\mathcal{L}} = P(\cap_{i\in\mathcal{L}} A_i \cap_{i\in\bar{\mathcal{L}}} \bar{A_i}).$$

Then $x_{\emptyset}$ is the probability that none of the events $A_1, ..., A_n$ occurs. On the other hand

$$P(\cup_{i=1}^{n} A_i) = \sum_{\emptyset\neq\mathcal{L}\subseteq\mathcal{N}} x_{\mathcal{L}}.$$

It is clear that the x values must satisfy the linear equations

$$\forall \emptyset \neq \mathcal{J} \in \mathcal{I}: \quad \sum_{\emptyset\neq\mathcal{J}\subseteq\mathcal{L}} x_{\mathcal{L}} = p_{\mathcal{J}} \tag{1}$$

and

$$\sum_{\mathcal{L}\subseteq\mathcal{N}} x_{\mathcal{L}} = 1. \tag{2}$$

If $\mathcal{I}$ does not contain all of the subsets of $\mathcal{N}$ then the equations (1), and (2) do not determine uniquely the values of x's. Thus only approximation can be given for the value of $P(\cup_{i=1}^{n} A_i)$. Taking into account that the probabilities are nonnegative quantities, $P(\cup_{i=1}^{n} A_i)$ is a value in the interval of the optimal values of the following two linear programming problems:

$$\begin{gathered} \max \sum_{\emptyset\neq\mathcal{L}\subseteq\mathcal{N}} x_{\mathcal{L}} \\ \forall \mathcal{J} \in \mathcal{I}: \sum_{\mathcal{J}\subseteq\mathcal{L}} x_{\mathcal{L}} = p_{\mathcal{J}} \\ \forall \mathcal{L} \subseteq \mathcal{N}: x_{\mathcal{L}} \geqslant 0, \end{gathered} \tag{3}$$

and

$$\begin{gathered} \min \sum_{\emptyset\neq\mathcal{L}\subseteq\mathcal{N}} x_{\mathcal{L}} \\ \forall \mathcal{J} \in \mathcal{I}: \quad \sum_{\mathcal{J}\subseteq\mathcal{L}} x_{\mathcal{L}} = p_{\mathcal{J}} \\ \forall \mathcal{L} \subseteq \mathcal{N}: \quad x_{\mathcal{L}} \geqslant 0. \end{gathered} \tag{4}$$

Regarding upper bounds the LP problem (3) is the important one. The optimal value of problem (3) may be greater than 1 if $\emptyset \notin \mathcal{I}$ as the problem does not contain constraint (2). In this case 1 is automatically taken as an upper bound.

In what follows it is assumed that $\mathcal{I}$ consists of all subsets of $\mathcal{N}$ having either 1 or 2 elements. For the sake of convenience the following notations are introduced. Let $1 \leqslant k, l \leqslant n$, $k \neq l$ be two arbitrary indices. Then $p_i = P(A_i)$ and p_{kl} denotes the probability that both A_k, and A_l occurs, i.e.

$$p_{kl} = P(A_k \cap A_l).$$

Then the appropriate form of (3) has

$$n + \binom{n}{2}$$

linear constraints and $2^n - 1$ variables. The coefficient of a variable $x_{\mathcal{L}}$ in a constraint belonging to the probability $p_{\mathcal{J}}$ is 1 if $\mathcal{J} \subseteq \mathcal{L}$, otherwise it is 0. Let us denote the variables of the dual of (3) by $\mathbf{y} = (y_1, ..., y_n, y_{12}, ..., y_{n-1,n})$. The vector $\mathbf{y}$ is feasible in the dual problem if and only if

$$\forall \emptyset \neq \mathcal{L} \subseteq \mathcal{N} : \sum_{i \in \mathcal{L}} y_i + \sum_{1 \leqslant i < j \leqslant n : \{i,j\} \subseteq \mathcal{L}} y_{ij} \geqslant 1. \tag{5}$$

Notice that the dual variables are not necessarily nonnegative. The objective function of the dual is

$$\min \sum_{i=1}^{n} p_i y_i + \sum_{1 \leqslant i < j \leqslant n} p_{ij} y_{ij} \tag{6}$$

The following notations are used throughout the paper:

$$S_1 = \sum_{i=1}^{n} p_i,$$

and

$$S_2 = \sum_{1 \leqslant i < j \leqslant n} p_{ij}.$$

3. Upper bounds based on graph structures: general properties

It is well-known in the theory of linear programming that the objective function value of any feasible solution of the dual problem (5)-(6) gives an upper bound to the optimal value of problem (3). Thus the underlying logic to find an upper bound for the probability of the union of events is to find a feasible solution of the dual problem is and to calculate its objective function value. Any bound obtained in this way will be called dual-type bound. In this section a large class of dual type bounds will be shown to have the following properties: (i) for some problems the probability of the union of events is equal to the upper bound, and (ii) the dual type bounds are always at least as good as the aggregated bound of [13].

In this paper feasible solutions of (5)-(6) will be considered only in the form:

$$\mathbf{y} = (1, 1, ..., 1, -w_{12}, ..., -w_{n-1,n}),$$

where the parameters $w_{12}, ..., w_{n-1,n}$ may take positive, negative, and zero values To each such feasible solution the objective function value (6) has the form

$$S_1 - \sum_{1 \leqslant i < j \leqslant n} w_{ij} p_{ij} \tag{7}$$

providing an upper bound to (3) and hence to $P(\cap_{i \in \mathcal{J}} A_i)$.

It is easy to see that the following statement holds:

LEMMA 1. *A vector* $\mathbf{y}^T = (1, 1, ..., 1, -w_{12}, ..., -w_{n-1,n})$ *satisfies the inequalities* (5) *if and only if for all* $\mathcal{L} \subseteq \mathcal{N}$ *containing at least two elements the inequality*

$$\sum_{i,j \in \mathcal{L},\, i<j} w_{ij} \leqslant | \mathcal{L} | -1 \tag{8}$$

is satisfied.

A graph $G(\mathcal{N}, E)$ can be defined by weights w_{ij} as $E = \{\{i,j\} | i < j,\ w_{ij} \neq 0\}$. Sometimes it will be advantageous to consider G as the union of two graphs, say $G^1 = (\mathcal{N}, E^1)$ and $G^2 = (\mathcal{N}, E^2)$ when $E^1 = \{\{i,j\} \mid i < j, w_{ij} > 0\}$, and $E^2 = \{\{i,j\} \mid i < j, w_{ij} < 0\}$.

The first bound which can be discussed in this framework is Hunter's bound (see Hunter [10]), which is the best bound of type (7) corresponding to spanning trees. Let $G^1 = T(\mathcal{N}, E^1)$ be any tree, and $G^2 = (\mathcal{N}, \emptyset)$. Let

$$w_{ij} = \begin{cases} 1 & \text{if } \{i,j\} \in E^1 \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

As the cardinality of edges is always less than the cardinality of vertices in any forest therefore the feasibility of the vector $\mathbf{y}^T = (1, 1, ..., 1, -w_{12}, ..., -w_{n-1,n})$ in (5) follows immediately if the weights are chosen according to (9). Thus

$$P\left(\cup_{i=1}^{n} A_i\right) \leqslant S_1 - \max_{\mathcal{T}(\mathcal{N},E):\mathcal{T} \text{ is a tree}} \sum_{\{i,j\} \in E^1} p_{ij}. \tag{10}$$

In Hunter's bound all positive weights are equal to 1. We shall consider upper bounds of type (7), in which similarly to Hunter's bound, we have all positive weights are equal to 1. The negative weights can be considered as compensation for the fact that the number of positive edges is greater than $n-1$, i.e. the number of positive weights in the Hunter bound.

3.1. Special cases when the bounds are equal to the exact value

THEOREM 1. *Assume that the vector* $(1, ..., 1, -w_{12}, ..., -w_{n-1,n})^T \in R^{\frac{n(n+1)}{2}}$ *is feasible in* (5). *Assume further on that all positive weights are equal to 1. Then there exists a problem instance such that the upper bound is equal to* $P(A_1 \cup ... \cup A_n)$.

Proof. The upper bound is

$$S_1 - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} p_{ij}.$$

Assume that each of the events $A_1, ..., A_n$ is the union of n mutually exclusive atomic events, say $A_j = \omega_{1j} \cup ... \cup \omega_{nj}$ for $j = 1, ..., n$. Assume that the probability of each ω_{ij} is $1/n^2$. Then the probability of A_j is $1/n$. We choose the atomic events in such a way that $\omega_{ij} \neq \omega_{kl}$ if $(i,j) \neq (k,l), (l,k)$. Hence it immediately follows that no three events out of $A_1, ..., A_n$ can occur at the same time, i.e. the sieve formula of the exact probability of $A_1 \cup ... \cup A_n$ does not contain terms with higher degree than 2. Finally let $\omega_{ij} = \omega_{ji}$ if and only if $w_{ij} = 1$. Now the following equation holds

$$P(A_1 \cup ... \cup A_n) = 1 - \frac{\sum_{i<j:w_{ij}=1} 1}{n^2} = S_1 - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} p_{ij},$$

i.e., the statement of the theorem is true. □

3.2. Average behavior

It is well-known that the formula

$$S_1 - \frac{2}{n} S_2 \tag{11}$$

is an upper bound for the probability of the union of the events $A_1, ..., A_n$, see e.g. [5], [13], [21]. It is an aggregated bound as there is no individual probability in the formula. In this subsection a general theorem is proved, which makes it easy to prove for a wide class of dual type upper bounds, that they are at least as good as the corresponding aggregated one, i.e. (11).

The underlying idea of the results of this subsection is as follows. The starting point is a complete graph K_n. A subgraph G of K_n is fixed. More precisely, fixing here concerns only the structure of G but the particular vertices and therefore the particular edges of G can be changed. If the "goodness" of G for any particular vertex set is measured by a real number, then the best vertex set must be at least as good as the average behavior of G.

THEOREM 2. *Let* $\mathcal{N}^1 = \{\{i,j\} \mid 1 \leqslant i < j \leqslant n\}$, $\mathcal{N}^2 = \{1,2,...,r\}$, *where* $r = \binom{n}{2}$, *and assume that the function* $\rho : \mathcal{N}^1 \to \mathcal{N}^2$ *defines a one-to-one correspondence between the two sets. Let* $w_1, ..., w_r$ *be any real numbers satisfying the equation*

$$\sum_{j=1}^{r} w_j = n - 1.$$

Finally, let π *be any permutation of the set* $\{1, ..., n\}$. *Then the following inequality holds:*

$$\max_{\pi:} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{\rho(i,j)} p_{(\pi(i),\pi(j))} \geqslant \frac{2}{n} S_2. \tag{12}$$

Proof. The left-hand side of the inequality is the maximum of a few numbers. The average of the same numbers is

$$\frac{1}{n!} \sum_{\pi:} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{\rho(i,j)} p_{(\pi(i),\pi(j))}.$$

The expression is symmetric implying that all p values must have the same coefficient in the sum, that is

$$\frac{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{\rho(i,j)}}{\binom{n}{2}} = \frac{2}{n},$$

as there are $n!$ permutations, the number of w's is $\binom{n}{2}$, and their sum is $n-1$. Thus, the above average is equal to the right-hand side of the inequality. Hence the statement follows immediately. □

REMARK. The proof does not use any particular properties of the p's, hence the statement holds for any vector $p \in R^{\frac{n(n-1)}{2}}$, and $S_2 = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} p_{ij}$.

In the statement the w values represent a fixed structure and the permutation of the p's ensures that the best sample is chosen that is isomorphic with the fixed structure. For example, the statement that Hunter's bound is at least as good as the aggregated bound, follows from the theorem in two steps. First, the vector w is fixed in such a way that it represents a certain tree structure. The best tree is selected that is isomorphic with this structure. Then, we look at all the tree structures and then the best of bests gives Hunter's bound. Then, it follows from the theorem that the best of any tree structure is at least as good as the aggregated bound.

Assume that the vector $(1,1,...,1,-w_1,...,-w_r^T) \in R^{r+n}$ represents a dual feasible solution to problem (3). Then the theorem is applicable and

$$S_1 - \max_{\pi:} \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{\rho(i,j)} p_{(\pi(i),\pi(j))} \leqslant S_1 - \frac{2}{n} S_2.$$

It will be proven at the end of the next section that the left-hand side is an upper bound for the probability in question.

4. Upper bounds based on graph structures: particular cases

In this section two rather general upper bounds are proven.

To understand the statement of theorem 3 a well-known notion of graph theory is required.

DEFINITION 1. Let (V,E) be an undirected graph. The sequence G_1, G_2, ..., G_k of subgraphs of G is an ear-decomposition of G if the following conditions hold:

(i) $G_1(V_1,E_1)$ is a circuit,

(ii) $G_i(V_i,E_i)$ is obtained from $G_{i-1}(V_{i-1},E_{i-1})$ by connecting two vertices of G_{i-1}, say u_i and v_i, by a path $P_i = \{\{u_i = w_1, w_2\},...,\{w_{l_i-1}, w_{l_i} = v_i\}\}$ such that $w_2,...,w_{l_i-1} \notin V_{i-1}$.

(iii) $G_k = G$.

It is well-known that a graph has an ear-decomposition if and only if it is 2-connected [7].

THEOREM 3. *Let $G(V,E)$ be a graph having an ear-decomposition $G_1,\dots,G_k$. Let $\mathcal{H} = \{\{u_1,v_1\},\dots,\{u_k,v_k\}\}$ be a multi-set, where $\{u_1,v_1\}$ is a chord of G_1 and $\{u_i,v_i\}$ is the pair of vertices connected by P_i. Assume that $\mathcal{H}\cap E=\emptyset$. Let*

$$w_{uv} = \begin{cases} 1 & \text{if } \{u,v\}\in E \\ -\#\text{ of appearances of } \{u,v\} \text{ in } \mathcal{H}, & \text{if } \{u,v\}\in\mathcal{H} \\ 0 & \text{otherwise.} \end{cases}$$

Then the following inequality holds:

$$P(A_1\cup\dots\cup A_n) \leqslant S_1 - \sum_{\{u,v\}:u<v} w_{uv}p_{uv}. \tag{13}$$

THEOREM 4. *Assume (a) that $C_1,\dots,C_t$ is a set of circuits of graph G, (b) the union of the edge sets of the circuits equals the set of edges of G, (c) each circuit $C_1,\dots,C_t$ has a length of at least 4. Let $\mathcal{H} = \{\{u_1,v_1\},\dots,\{u_t,v_t\}\}$ be a multi-set of chords of circuits such that $\{u_j,v_j\}$ belongs to C_j $(j=1,\dots,t)$. Let*

$$w_{uv} = \begin{cases} 1 & \text{if } \{u,v\}\in E \\ -\#\text{ of appearances of } \{u,v\} \text{ in } \mathcal{H} & \text{if } \{u,v\} \text{ is a chord} \\ 0 & \text{otherwise.} \end{cases}$$

Then we have the inequality:

$$P(A_1\cup\dots\cup A_n) \leqslant S_1 - \sum_{\{u,v\}:u<v} w_{uv}p_{uv}. \tag{14}$$

REMARKS: 1. It is clear that the right-hand sides of (13), and (14) are equal to

$$S_1 - \sum_{\{u,v\}\in E,u<v} p_{uv} + \sum_{i=1}^{k} p_{u_iv_i}$$

and

$$S_1 - \sum_{\{u,v\}\in E,u<v} p_{uv} + \sum_{i=1}^{t} p_{u_iv_i},$$

respectively.

2. The theorems give the following two upper bounds:

$$P(A_1\cup\dots\cup A_n) \leqslant S_1 - \max_{\substack{G_1,\dots,G_k \text{ is an} \\ \text{ear-decomposition}}} \left(\sum_{\{p,q\}\in E,p<q} p_{pq} - \sum_{i=1}^{m} p_{u_iv_i} \right) \tag{15}$$

and

$$P(A_1\cup\dots\cup A_n) \leqslant S_1 - \max_{\substack{\mathcal{H} \text{ is a multi-} \\ \text{set of chords}}} \left(\sum_{\{p,q\}\in E,p<q} p_{pq} - \sum_{i=1}^{m} p_{u_iv_i} \right) \tag{16}$$

Proof of theorems 3 *and* 4. The proofs of the two theorems are based on the same observations. First of all we remark that the $n+\binom{n}{2}$ -component vector

$$\mathbf{y}=(1,1,...,1,-w_{12},...,-w_{n-1,n}) \tag{17}$$

is feasible in the dual problem, i.e. it satisfies (5), if and only if for all $S\subseteq\mathcal{N}$ containing at least two elements the inequality

$$\sum_{i,j\in S,\, i<j} w_{ij}\leqslant\mid S\mid -1 \tag{18}$$

holds. The following construction is a direct application of this fact. Let $G^1(\mathcal{N},E^1)$ and $G^2(\mathcal{N},E^2)$ be two graphs on the vertex set $\mathcal{N}$. Assume that to each $\{i,j\}$, $i,j\in\mathcal{N},\ i\neq j$ a real number w_{ij} is assigned and the following conditions are satisfied:

(i) $E^1\cap E^2=\emptyset$,

(ii) if $\{i,j\}\in E^1$ then $w_{ij}=1$,

(iii) if $\{i,j\}\in E^2$ then $w_{ij}\leqslant 0$,

(iv) if $\{i,j\}\notin E^1\cup E^2$ then $w_{ij}=0$,

(v) if $\mathcal{S}\subseteq\mathcal{N},\mid\mathcal{S}\mid\geqslant 2$, then $\sum_{i,j\in\mathcal{S},\, i<j} w_{ij}\leqslant\mid S\mid -1$.

Then

$$P(A_1\cup...\cup A_n)\ \leqslant S_1-\sum_{\{i,j\}\in E^1} p_{ij}+\sum_{\{i,j\}\in E^2}(-w_{ij})p_{ij}. \tag{19}$$

The case of Theorem 3. Assume that the graph G has the ear-decomposition G_1, G_2,... G_k as it is given in Definition 1. The weights of the edges are determined iteratively. A new ear is added to the graph in each iteration. G_1 is a circuit. Let all of its edges have weight 1 and the weight of the chord (u_1,v_1) is -1. The weight of all other edges is 0 at the end of the first iteration. Then condition (19) holds. Let us assume that (19) is satisfied after iteration l. In iteration $l+1$ a path called P_{l+1} is added to the graph. P_{l+1} connects the two vertices of G_l, say u_{l+1} and v_{l+1}, and all other vertices of P_{l+1} are vertices not contained in G_l. In iteration $l+1$ the weight of the edges of P_{l+1} are changed from 0 to 1, and the weight of (u_{l+1},v_{l+1}) is decreased by 1. Let the weight of the pair of vertices $\{i,j\}$ be denoted at the end of iteration l by w_{ij}^l.

Let $\mathcal{S}$ be a set of vertices. Notice that only the following pairs of vertices $\{i,j\}$ may have a weight w_{ij}^{l+1} different from zero in $\mathcal{S}$:

– $\{u_{l+1},v_{l+1}\}$ if $u_{l+1},v_{l+1}\in\mathcal{S}$,

– the edges of P_{l+1} having weight 1,

– any $\{i,j\}\in\mathcal{S}\setminus(P_{l+1}\setminus\{u_{l+1},v_{l+1}\})$.

Let $\mathcal{E}(P_{l+1})$ be the edge set of P_{l+1}. Then the sum of weights of the pairs of $\mathcal{S}$ can be determined after iteration $l+1$ on the following way.

First assume that $u_{l+1}, v_{l+1} \in \mathcal{S}$. Then

$$\sum_{i,j\in\mathcal{S},i<j} w_{ij}^{l+1} = \sum_{\substack{i,j\in\mathcal{S}\setminus(P_{l+1}\setminus\{u_{l+1},v_{l+1}\}),\\ i<j}} w_{ij}^{l} \quad -1+ \sum_{\substack{i,j\in\mathcal{S}\\ (i,j)\in\mathcal{E}(P_{l+1}),\\ i<j}} 1$$

$$\leqslant |\mathcal{S}\setminus(P_{l+1}\setminus\{(u_{l+1},v_{l+1})\})|-1-1+|\mathcal{S}\cap(P_{l+1}\setminus\{(u_{l+1},v_{l+1})\})|+1=|\mathcal{S}|-1,$$

where after the first equation -1 stands for the decrease of the weight of the pair (u_{l+1}, v_{l+1}) and the $+1$ after the inequality stands for the two possible edges of $\mathcal{S}\cap P_{l+1}$ connecting u_{l+1} and v_{l+1}, respectively, to the other part of P_{l+1}. If at most one of u_{l+1}, v_{l+1} is in $\mathcal{S}$, then

$$\sum_{i,j\in\mathcal{S},i<j} w_{ij}^{l+1} = \sum_{\substack{i,j\in\mathcal{S}\setminus(P_{l+1}\setminus\{u_{l+1},v_{l+1}\}),\\ i<j}} w_{ij}^{l} \quad + \sum_{\substack{i,j\in\mathcal{S}\\ (i,j)\in\mathcal{E}(P_{l+1}),\\ i<j}} 1$$

$$\leqslant |\mathcal{S}\setminus(P_{l+1}\setminus\{(u_{l+1},v_{l+1})\})|-1+|\mathcal{S}\cap(P_{l+1}\setminus\{(u_{l+1},v_{l+1})\})|=|\mathcal{S}|-1.$$

Hence (19) holds.

The case of Theorem 4. Any subgraph of G^1 induced by a set $\mathcal{S}\subseteq\mathcal{N}$ contains at most $|\mathcal{S}|-1+r$ edges, where r is the number of circuits, with vertices contained completely in $\mathcal{S}$. The necessary inequality given in the construction holds because there are r edges of type $\{u_i, v_i\}$ counted with multiplicity and having weight -1. □

Theorem 4 is a generalization of the next two theorems as in the case of these the length of the circuit G_1 is 4 and the length of all P_i paths is 2 and all of them connect two points in a fixed subset of vertices.

THEOREM 5. ([20]; lemma 6.2) *Assume that* $n\geqslant 3$. *Let* k, *and* l *be two indices such that* $1\leqslant k<l\leqslant n$. *Let* $\mathcal{T}\subseteq\{1,...,n\}\setminus\{k,l\}$ *be an arbitrary index set. Then*

$$P(A_1\cup...\cup A_n)\leqslant S_1-\sum_{i\in\mathcal{T}}(p_{ik}+p_{li})+(|\mathcal{T}|-1)p_{kl}. \tag{20}$$

This statement was later generalized ([22]; Proposition 2.1.7) in the following way:

THEOREM 6. *Let* $\mathcal{A}$, *and* $\mathcal{B}$ *two disjoint subsets of* $\mathcal{N}$. *Then*

$$P(A_1\cup...\cup A_n)\leqslant S_1-\sum_{i\in\mathcal{A}}\sum_{k\in\mathcal{B}}p_{ik}+(|\mathcal{A}|-1)\sum_{k,l\in\mathcal{B},k\neq l}p_{kl}. \tag{21}$$

This theorem can be generalized further on by the following heuristic algorithm. Let $\mathcal{B}$ be a subset of $\mathcal{N}$ such that $|\mathcal{B}|\geqslant 2$, and $\mathcal{A}=\mathcal{N}\setminus\mathcal{B}\neq\emptyset$. It is better to choose set $\mathcal{B}$ such that

$$\frac{1}{\binom{|\mathcal{B}|}{2}}\sum_{i<j;i,j\in\mathcal{B}}p_{ij}<\frac{1}{\binom{n}{2}}\sum_{1\leqslant i<j\leqslant n}p_{ij}.$$

In the initial step all weights are 0. Then for all triplets (i,j,k) such that $i,j\in\mathcal{B}$ $(i<j)$, and $k\in\mathcal{A}$ if

$$p_{ik}+p_{jk}>p_{ij},$$

then define

$$w_{ij} := w_{ij} - 1, w_{ik} = w_{jk} = 1.$$

Finally denote

$$(i^*, j^*) = \text{argmin}\,\{p_{ij} | i,j \in \mathcal{B};\ i < j\},$$

and

$$w_{i^*j^*} := w_{i^*j^*} + 1.$$

The next lemma is a tool to generate overall upper bounds from locally small ones.

LEMMA 2. *Let $G^1(V^1, E^1)$, and $G^2(V^2, E^2)$ be two undirected graphs having at most one vertex in common. Assume that the vectors $\mathbf{w}^1$, and $\mathbf{w}^2$ of type (17) satisfy the appropriate condition (18). Then the vector $\mathbf{w} = (\mathbf{w}^1, \mathbf{w}^2)$ satisfies (17) in the graph $G(V^1 \cup V^2, E^1 \cup E^2)$, too.*

Proof. Let us have $S \subseteq V^1 \cup V^2$, $S^1 = S \cap V^1$ and $S^2 = S \cap V^2$. If $|S^1| \leqslant 1$ or $|S^2| \leqslant 1$ then the inequality (18) for S coincides with one of the inequalities for S^2 or S^1, respectively. Otherwise the inequality for S can be obtained from the sum of the inequalities of the two subsets. □

The Hunter bound can be improved by the following heuristic algorithm. The algorithm works on the complete graph $K_n(\mathcal{N}, E)$. Let p_{ij} be the weight of the edge $\{i,j\}$ of K_n.

Step 1: Find a maximum weight spanning tree of K_n, denote it by $T(\mathcal{N}, E_T)$.

Step 2: For any edge $\{i,j\} \in E \setminus E_T$ let $C_{ij} = \{\{u_1^{ij}, u_2^{ij}\}, \dots, \{u_{l_{ij}-1}^{ij}, u_{l_{ij}}^{ij}\}, \{u_{l_{ij}}^{ij}, u_1^{ij}\}\}$ be the unique simple circuit of the graph $T_{ij}(\mathcal{N}, E_T \cup \{i,j\})$, where l_{ij} is the length of C_{ij}. Then, let us denote

$$(i^*, j^*, s^*, t^*) = \text{argmax}\,\{p_{ij} - p_{st} : l_{ij} \geqslant 4, 1 \leqslant s < t \leqslant l_{ij}, t - s \not\equiv \pm 1 \bmod l_{ij}\}. \quad (22)$$

If $p_{i^*j^*} - p_{s^*t^*} > 0$, then the resulting bound based on the graphs $G = T_{i^*j^*}$ and $G^2(\mathcal{N}, \{s^*, t^*\})$ is an improvement on Hunter's bound. The order of the algorithm is $O(n^4)$. In (22) the number of pairs $\{i,j\}$ to be considered is $O(n^2)$. The determination of C_{ij} is equivalent to finding the unique simple path leading from i to j in T, and this can be done in $O(n)$ steps as the sum of the degrees of the vertices in T is $2n-2$. Then, the selection of the best possible pair $\{s^*, t^*\}$ takes $O(n)$ operations.

A special case of this upper bound is obtained by restricting G^1 to a Hamiltonian circuit. Let $\mathcal{H}$ be the set of all Hamiltonian circuits. In this way the following upper bound can be obtained:

$$P(A_1 \cup \ldots \cup A_n) \leqslant S_1 - \max_{H \in \mathcal{H}} \left(\sum_{\{i,j\} \in H, i<j} p_{ij} - \min_{\{s,t\} \notin H} p_{st} \right). \quad (23)$$

The second term of the right-hand side is equivalent to a traveling salesman problem which is known to be NP-hard. But plenty of good and fast heuristics are available to generate approximate solutions.

COLLORARY 1. *Assume that the vector* $(1,1,...,1,-w_1,...,-w_r^T) \in R^{r+n}$ *represents a dual feasible solution to problem* (3). *Then*

$$P(A_1 \cup ... \cup A_n) \leqslant S_1 - \max_{\pi:} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{\rho(i,j)} p_{(\pi(i),\pi(j))}$$

Proof. The vector $(1,1,...,1,-w_1,...,-w_r^T)$ is dual feasible if and only if (18) is true for all subsets $S \subseteq \mathcal{N}$. Any permutation π of the vertices defines a one-to-one correspondence of the subsets of $\mathcal{N}$ such that any subset is mapped into a subset of the same cardinality. Furthermore the edges of the subgraph induced by S are mapped into the edges of the subgraph induced by $\pi(S)$. Hence (18) remains true.

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