COMBINATORICA Bolyai Society – Springer-Verlag

BICLIQUES IN GRAPHS I: BOUNDS ON THEIR NUMBER

ERICH PRISNER

Received January 27, 1997

Abstract. Bicliques are inclusion-maximal induced complete bipartite subgraphs in graphs. Upper bounds on the number of bicliques in bipartite graphs and general graphs are given. Then those classes of graphs where the number of bicliques is polynomial in the vertex number are characterized, provided the class is closed under induced subgraphs.

1. Introduction

Inclusion-maximal induced complete bipartite graphs are called bicliques. This notion may be considered as a bipartite graph analogue of the notion of clique (i.e. maximal complete subgraphs). Besides being rather natural, investigating bicliques in graphs or bipartite graphs, and looking for bounds on their number is interesting for two reasons. Firstly, they are the key structure in intersection bigraphs [5],[9],[12] in underlying graphs of intersection digraphs [7], [13], and even in some other 'geometrically defined' graphs [3], [6]. In most cases, some (few) bicliques encode most of the information about the original structure. Therefore, generating all bicliques and sampling the information seems a promising approach for recognition algorithms, as will be shown in a subsequent paper for certain 2-path graphs and certain underlying graphs of line digraphs [11]. Secondly, finding a 'largest' (with respect

Mathematics Subject Classification (1991): 05C

Supported by the Deutsche Forschungsgemeinschaft under grant no. Pr 324/6-1; part of this research was done at Clemson University, whose hospitality is greatly acknowledged.

to vertex or edge number or weight, for instance) induced complete bipartite subgraph is trivially polynomial if the number of bicliques is polynomial in the vertex number. For triangle-free graphs, this is just the well-known problem of finding 'large' not-necessarily induced complete bipartite graphs, see [4], problems GT24 or GT25.

Note that we even view edgeless graphs as complete bipartite graphs $K_{a,0}$. Since therefore all maximal independent sets occur as partition sets of bicliques, the concept may also be viewed as an extension of the notion of maximal independent sets. However, for some applications we are only interested in bicliques where both partition sets contain enough elements. A biclique is said to have $type \geq k$ if both partition sets contain at least k elements (i.e., if the biclique contains $K_{k,k}$).

Before outlining the contents of the paper, let us first introduce several classes of graphs which play an important role in this paper:

- 1) The join G*H of two graphs G and H is obtained from their disjoint union by joining every vertex of G with every vertex of H by an edge. For disjoint sets U and W, U*W denotes the complete bipartite graph with bipartition U and W. Bicliques in G*H have either the form U_1*U_2 , where U_1 and U_2 are maximal independent sets in G and H respectively, or they are the bicliques of type ≥ 1 in G or H, respectively.
- 2) The cocktail party graph CP(j) of order j is obtained from the complete bipartite graph $K_{j,j} = jK_1 * jK_1$ by deleting some perfect matching. Note that $CP(3) = C_6$, and that CP(4) is just the ordinary cube graph. Let $V(CP(j)) = \{a_1, a_2, \ldots, a_j, b_1, b_2, \ldots, b_j\}$ and $E(CP(j)) = \{a_i b_p : i \neq p\}$. Induced bicliques of CP(j) have just the form $\{a_i : i \in I\} \cup \{b_p : p \in \{1, 2, \ldots, j\} \setminus I\}$ for subsets I of $\{1, 2, \ldots, j\}$. Therefore there are just 2^j of them.
- 3) The graph $H(k,\ell) = kK_1 * \ell K_2$ contains 2^{ℓ} induced bicliques, all of them $K_{k,\ell}$ s. The graphs $H(1,\ell)$ are known under the name friendship graphs.

We give examples in Figure 1. All graphs in this figure have 10 vertices. CP(5) is bipartite with $2^5 = 32$ bicliques. H(2,4) contains $2^4 = 16$ bicliques of type ≥ 2 and 4 further bicliques of type ≥ 1 . Finally, $(K_3 \cup K_2) * (K_3 \cup K_2)$ contains $2^2 3^2 = 36$ bicliques of type ≥ 2 , and 8 further bicliques of type ≥ 1 .

In Section 2 we investigate the maximum number of bicliques in graphs and bipartite graphs— as already mentioned, they are exponential in the vertex number. In Section 3 we give bounds on the number of bicliques in CP(j)-free bipartite graphs, respectively bicliques of type $\geq k$ in general CP(j)-free and $H(k,\ell)$ -free graphs, that are polynomial in the vertex number and only exponential in the constants j,k,ℓ . Such bounds are important, since they are the reason why polynomial-time recognition algorithms for interval bigraphs or interval digraphs [9], certain line bigraphs [12], underlying

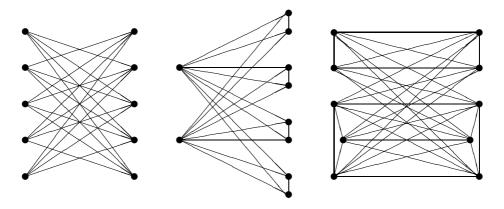


Fig. 1. The graphs CP(5), H(2,4), and $(K_3 \cup K_2) * (K_3 \cup K_2)$.

graphs of line digraphs of minimum degree high enough, or 2-path graphs of graphs of high enough minimum degree [11] are possible. In all these examples the algorithms include the generation of all bicliques whose type exceeds a certain number.

2. Exponential bounds

Since the vertex sets of bicliques are distinct and noncomparable by inclusion, Sperner's Lemma implies an upper bound of $\binom{n}{\lfloor n/2 \rfloor}$ for the number of bicliques in an *n*-vertex graph, which is approximately $\sqrt{\frac{2}{\pi n}}2^n$ by Stirling's formula. For bipartite graphs we can do much better:

Theorem 2.1. Every bipartite graph with n vertices contains at most $2^{n/2} \approx 1.41^n$ bicliques, and the only extremal bipartite graphs are the graphs CP(k).

Proof. Let $B = (U \cup W, E)$ be bipartite, with w.l.g. $|U| \leq |W|$. We may generate all bicliques in the following way. Starting with any subset $Z \subseteq U$, we look at $Z' = \bigcap_{x \in Z} N(x) \subseteq W$. Taking $Z'' = \bigcap_{y \in Z'} N(y)$, Z'' * Z' forms a biclique in B. Obviously, every biclique X * Y occurs in this way, since X' = Y and Y' = X then. Since there are $2^{|U|}$ subsets of U, there are at most $2^{|U|} \leq 2^{n/2}$ bicliques. Equality implies |U| = |W|, and that all these bicliques generated are distinct. Then $Z \neq Y \subseteq U$ must imply $Z' \neq Y'$. Certainly $Z \subseteq Y$ implies $Z' \supseteq Y'$, therefore, in the case of $2^{n/2}$ bicliques, the mapping $Z \to Z'$ is an anti-order-isomorphism between $(\mathcal{P}(U), \subseteq)$ and $(\mathcal{P}(W), \subseteq)$. This implies

that for every $x \in U$ there must be some $x' \in W$ such that $\{x\}' = W \setminus \{x'\}$. Then we have B = CP(n/2).

In the nonbipartite case, $3^{n/3} \approx 1.44^n$ bicliques, even of large type, are possible, as can be seen by the graphs $\lfloor m \rfloor K_3 * \lceil m \rceil K_3$ (Slightly worse numbers are achieved by the graphs $(K_4 \cup \lfloor m \rfloor K_3) * \lceil m \rceil K_3$ if $n \equiv 1 \mod 3$, or by $(K_2 \cup \lfloor m \rfloor K_3) * \lceil m \rceil K_3$ if $n \equiv 2 \mod 3$). A compromise between the trivial upper bound 2^n and the lower bound 1.44^n for the worst case is the following bound, where surprisingly the golden ratio occurs:

Theorem 2.2. Every graph with n vertices contains at most

$$n^{5/2}(1.618034^n + o(1))$$

bicliques.

Proof. We count the number of bicliques of G containing a given edge xy. We define $U = N(y) \setminus N(x)$ and $W = N(x) \setminus N(y)$, where w.l.g. $|U| \le |W|$. Every such biclique of type ≥ 2 must w.l.g. have the form $(S \cup \{x\}) * (T \cup \{y\})$ with $S \subseteq U$ and $T \subseteq W$.

Let $U' \cup \{x\} * W' \cup \{y\}$ be a largest biclique (with respect to number of vertices).

Every further biclique $S \cup \{x\} * T \cup \{y\}$ is uniquely determined by the pair $S \setminus U'$ and $T \setminus W'$ as follows: Elements of $S \cap U'$ must be adjacent to all vertices in $T \setminus W'$, and nonadjacent to all vertices of $S \setminus U'$. We get

$$S \cap U' \subseteq U' \cap \bigcap_{w \in T \setminus W'} N(w) \setminus \bigcup_{u \in S \setminus U'} N(u), \text{ and}$$

 $T \cap W' \subseteq W' \cap \bigcap_{u \in S \setminus U'} N(u) \setminus \bigcup_{w \in T \setminus W'} N(w).$

Since every element of U' is adjacent to every element of W', we get equality in both cases.

Let us abbreviate $\lambda = \frac{|U' \cup W'|}{|U \cup W|}$, and $m = |U \cup W|$. We distinguish two cases:

Case 1. $\lambda \ge \frac{1}{3}$. Then a rough estimate will do. The number of bicliques containing the edge xy is at most

$$2^{|U\setminus U'|}2^{|W\setminus W'|} = 2^{(1-\lambda)m} \le 2^{2m/3} \le 2^{2n/3} \approx 1.587^n$$
.

Case 2. $\lambda \leq \frac{1}{3}$. The number of bicliques containing the edge xy is at most

$$\sum_{a=0}^{|U' \cup W'|} \sum_{b=0}^{|U' \cup W'|-a} \binom{|U \setminus U'|}{a} \binom{|W \setminus W'|}{b}$$

$$(1) \qquad \qquad = \sum_{t=0}^{|U' \cup W'|} \binom{|U \cup W| - |U' \cup W'|}{t}$$

by Vandermonde's convolution. Note that the binomial coefficients occurring are not too big. This is since the lower index is small if $|U' \cup W'|$ is small, and since the upper index is small if $|U' \cup W'|$ is large.

Let t_0 denote the value where the binomial coefficient on the right of (1) is largest. Since $\lambda < \frac{1}{3}$, the maximum value for the binomial coefficients on the right of (1) is achieved for $t = \lambda m$. The value of (1), i.e. the upper bound for the number of bicliques containing xy is at most

$$\lambda m \binom{(1-\lambda)m}{\lambda m}.$$

By Stirling's formula, this is approximately

$$\lambda m \sqrt{\frac{(1-\lambda)m}{2\pi\lambda m(1-2\lambda)m}} \frac{((1-\lambda)m)^{(1-\lambda)m}}{(\lambda m)^{\lambda m}((1-2\lambda)m)^{(1-2\lambda)m}} \\ \leq \sqrt{\frac{m}{2\pi}} \left(\frac{(1-\lambda)^{1-\lambda}}{\lambda^{\lambda}(1-2\lambda)^{1-2\lambda}}\right)^{m}.$$

The function

$$f(\lambda) = \frac{(1-\lambda)^{1-\lambda}}{\lambda^{\lambda} (1-2\lambda)^{1-2\lambda}}$$

has derivative

$$f'(\lambda) = \ln(\frac{(1-2\lambda)^2}{\lambda(1-\lambda)})f(\lambda),$$

which achieves its maximum for $\lambda = \frac{5-\sqrt{5}}{10} \approx 0.2764$. The maximum value of f is about 1.618034.

Both in case 1 and in case 2, there are at most

$$\sqrt{\frac{n}{2\pi}}1.618034^n + o(1)$$

bicliques of G that contain the edge xy. Overall, there are at most $n^{5/2}(1.618034^n + o(1))$ bicliques in G. (Note that every biclique is counted as often as its edge number, however taking care of that could improve the bound only by a factor of $n^2/4$.)

A slightly different proof, yielding a slightly worse bound, goes as follows: There are at most $2^{|U|}$ candidates for the set $S \setminus \{x\}$. (Actually only the independent subsets of U are candidates for $S \setminus \{x\}$. But if $S_1 \subseteq S_2$ for such bicliques S_1*T_1 and S_2*T_2 , then there are further restrictions on T_1 —namely it must contain some element of $\bigcap_{s \in S_1} N(s) \cap W \setminus \bigcap_{s \in S_2} N(s)$.) For fixed S, every $T \setminus \{y\}$ must be a maximal independent set in the graph induced by $\bigcap_{s \in S} N(s) \cap W$. As a graph with at most |W| vertices, it contains at most $3^{|W|/3}$ maximal independent sets, by the MOON/MOSER result [8]. (This part seems also improvable, since the sets $\bigcap_{s \in S} N(s) \cap W$ must in general be smaller than W.) Therefore the number of bicliques of G of type ≥ 2 is at most

$$n^2 2^{|U|} 3^{|W|/3} \le n^2 2^{(n-2)/2} 3^{(n-2)/6} = n^2 (2^{1/2} 3^{1/6})^{n-2} \approx n^2 1.70^{n-2}.$$

Since there are at most $n3^{(n-1)/3}+3^{n/3}$ remaining bicliques, we get an upper bound of $(n^2+n+1)1.7^n$ for the number of bicliques.

3. Polynomial bounds

Interval bigraphs contain only few bicliques, since $C_6 = CP(3)$ is forbidden as an induced subgraph [9]. In trying to generalize this, let us consider forbidden induced cocktail party graphs. For the bipartite case, we add the requirement that $2K_1$ is only called a CP(1) if its two vertices lie in different bipartition sets.

Theorem 3.3. For every integer j, if the bipartite graph $B = (U \cup W, E)$ does not contain any induced CP(j), then it contains at most $(|U||W|)^{j-1}$ bicliques.

Proof. The proof is by induction over j. The case j=1 is obvious, since every CP(1)-free bipartite graph is complete bipartite, and therefore has only one biclique. So assume in what follows $j \geq 2$ and the validity of the statement for j-1. When we refer to a biclique as U'*W', we mean that U' and W' are its vertices in U and W respectively.

We form the weighted intersection graph Ω of the set of all bicliques of B. That is, the vertices of Ω are the bicliques of B, and two such vertices are joined by an edge if the corresponding bicliques have nonempty intersection. The edge is weighted by the number of vertices in the intersection. Then we choose some maximum spanning tree T in Ω . Let the bicliques $U_1 * W_1$ and $U_2 * W_2$ be adjacent in T. W.l.g. $U_1 \neq U_2$, and w.l.g. we can find $u \in U_1 \setminus U_2$. By the maximality of $U_2 * W_2$, there is some $w \in W_2 \setminus W_1$ not adjacent to u.

The union of N(u) and N(w) induces some bipartite graph, which we call B(u, w).

The graph $(U_1 \cap U_2) * (W_1 \cap W_2)$ is complete bipartite. It is not a biclique in B, but we shall show that it is a biclique in B(u,w). Assume not, then there is some biclique U' * W' of B(u,w) properly containing it, i.e. w.l.g. $U_1 \cap U_2 \subseteq U'$ and $W_1 \cap W_2 \subset W'$. Vertex u is adjacent to all vertices in W', and w to all vertices in U'. Therefore both $(U' \cup \{u\}) * W'$ and $U' * (W' \cup \{w\})$ are complete bipartite graphs in B, thus they are contained in bicliques C and D of B, respectively. All three pairs $(U_1 * W_1, C), (C, D)$, and $(D, U_2 * W_2)$ have more vertices in common than $U_1 * W_1$ and $U_2 * W_2$, a contradiction to the maximum spanning tree property of T in Ω .

Note also that B(u,w) is CP(j-1)-free—the union of every induced CP(j-1) in B(u,w) and $\{u,w\}$ would induce a CP(j) in B. By induction hypothesis, there are at most $(|U||W|)^{j-2}$ bicliques in B(u,w).

No distinct edges (U_1*W_1,U_2*W_2) and (U_3*W_3,U_4*W_4) of T can result in the same pair (u,w) and the same biclique $(U_1\cap U_2)*(W_1\cap W_2)$ in B(u,w). For, assume some do, and assume w.l.g. $u\in U_1,U_3$, and $w\in W_2,W_4$. Then $U_1\cap U_3\supseteq U_1\cap U_2\cup \{u\},\ W_1\cap W_3\supseteq W_1\cap W_2,\ U_2\cap U_4\supseteq U_1\cap U_2$, and $W_2\cap W_4\supseteq W_1\cap W_2\cup \{w\}$. Then U_1*W_1 and U_3*W_3 , as well as U_2*W_2 and U_4*W_4 are joined by heavier edges in Ω than both pairs U_1*W_1,U_2*W_2 , and $U_3*W_3,\ U_4*W_4$. Now choose some shortest path C_0,C_1,\ldots,C_t on T, connecting the edge (U_1*W_1,U_2*W_2) and the edge (U_3*W_3,U_4*W_4) , w.l.g. $C_0=U_1*W_1$. Deleting the edge (U_1*W_1,U_2*W_2) and adding the edge (U_2*W_2,U_4*W_4) in T would yield a spanning tree in Ω of larger weight than T, a contradiction.

Therefore different edges (U_1*W_1, U_2*W_2) in T have different encodings $(u, w, (U_1 \cap U_2)*(W_1 \cap W_2))$. We may assume that B contains at least one edge, therefore the number of edges of T is at most the number of possible encodings, i.e. at most $(|U||V|-1)(|U||V|)^{j-2} \leq (|U||V|)^{j-1}-1$. But the number of bicliques of B equals the edge number of T plus one, as desired.

Corollary 3.1. Let a class Γ of bipartite graphs be closed under induced subgraphs. Then there is some polynomial f(n) such that every member G = (V, E) of the class contains at most f(|V|) bicliques if and only if there is some $j \in \mathbb{N}$ such that $CP(j) \notin \Gamma$.

Hence bicliques and cocktail party graphs have the same relation for bipartite graphs, as cliques and generalized octahedra for graphs, see [1] and [10].

Theorem 3.4. For all integers j, k, ℓ , if G = (V, E) does not contain induced CP(j)s and induced $H(k, \ell)s$, then G contains at most $\frac{1}{(k!)^2}(\frac{|V|}{2})^{2k+2j+4\ell-2}$ bicliques of type $\geq k$.

Proof. We count the number of bicliques of type $\geq k$ containing a given induced $K_{k,k}$ with bipartition X and Y. Let the partition classes of such a biclique be $U \cup X$ and $W \cup Y$. Let X' denote the set of vertices outside X adjacent to every vertex of Y but to no vertex of X, and in the same way $Y' = \bigcap_{x \in X} N(x) \setminus \bigcup_{y \in Y} N[y]$. Then $U \subseteq X'$ and $W \subseteq Y'$, and U * W is a biclique in $G[X' \cup Y']$. Moreover, U and W must be contained in one of the maximal independent sets in X' respectively Y'. Since $H(k,\ell) \not\sqsubseteq G$, both sets X' and Y' induce ℓK_2 -free graphs. According to results in [1] and [10], the induced subgraphs contain at most $|X'|^{2\ell}$ respectively $|Y'|^{2\ell}$ maximal independent sets. But for maximal independent sets A in G[X'] and B in G[Y'], since $A \cup B$ induces a CP(j)-free bipartite graph, by Theorem 3.3 there are at most $(|A||B|)^{j-1}$ bicliques inside. Therefore, at most $|X'|^{2\ell}|Y'|^{2\ell}|A|^{j-1}|B|^{j-1} \le |X'|^{2\ell+j-1}|Y'|^{2\ell+j-1}$ bicliques of G contain this particular $K_{k,k}$. Under the restriction $|X'|+|Y'| \le |V|-2k$, this function achieves its maximum for $|X'|=\lfloor \frac{|V|-2k}{2} \rfloor$ and $|Y'|=\lceil \frac{|V|-2k}{2} \rceil$. By [2], there are at most $\binom{|V|/2}{k} \binom{|V|/2}{k}$

Corollary 3.2. Let Γ be a class of graphs that is closed under induced subgraphs, and let k be an integer. Then there is some polynomial f(n) such that every member G = (V, E) of the class contains at most f(|V|) bicliques of type $\geq k$ if and only if CP(j) and $H(k, \ell)$ do not lie in Γ for some integers j and ℓ .

4. Tricliques and so on

Vertices form a biclique in a graph G if and only if they are maximal with the property that they induce the vertex-disjoint union of two complete graphs in the complement \overline{G} of G. Thus we may define a triclique in G as a maximal vertex set inducing the vertex disjoint union of three complete graphs in \overline{G} . It has $type \geq k$ if every one of these three complete graphs contains at least k vertices. Tricliques lack applications like bicliques, but it seems likely that the results of the paper carry over—only with three families of obstructions now, namely $K_{j,j,j} - jK_3$, $kK_1 * CP(j)$, and $K_{k,k} * \ell K_2$. These graphs have 3^j , 2^j , or 2^ℓ tricliques of type $\geq k$, respectively, for $j, \ell \geq k$.

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Erich Prisner

Mathematisches Seminar, Universität Hamburg, Bundesstr. 55, 20146 Hamburg, Germany, ms6a013@math.uni-hamburg.de