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On Problem of Finding all Maximal Induced Bicliques of Hypergraph

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Abstract. The problem of finding all maximal induced bicliques of a hypergraph is considered in this paper. Theorem on connection between induced bicliques of the hypergraph H and corresponding vertex graph $L_2(H)$ is proved. An algorithm for finding all maximal induced bicliques is proposed. Results of computational experiments with the use of the proposed algorithm are presented.

Keywords: hypergraph, maximal induced bicliques, search algorithm.

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A hypergraph is an extension of classical graph in which an edge of a graph can join any number of vertices. Traditionally hypergraphs have found practical application in the development of relational databases and combinatorial chemistry [1, 2]. Ability to combine multiple vertices in one edge provides a powerful tool to study processes in various networks. Thus, hypergraphs are actively used in modelling road and telecommunication networks [3, 4]. They are also used for constructing semantic networks when processing texts in natural languages [5, 6].

Many problems in studies of such networks are reduced to problems of determining various configurations. Configuration means any system of subsets of a finite set [2]. Of particular interest are problems of enumeration type [2], in which the existence of configurations is beyond doubt but there are two problems: find the number of configurations and the method of their representation. Considering that networks are representable by hypergraphs the search for configurations can be conveniently formulated in the language of $(0, 1)$-matrices [3]. In this case, the problem of finding all maximal induced bicliques of hypergraph can be reduced to the problem of constructing complete submatrices [4]. Let us note that problems of finding such configurations are $\sharp P$-complete [5].

The problem of finding all maximal induced bicliques for each given hypergraph, which is called Maximal Induced Biclique Generation Problem for Hypergraphs (MIBGP for Hypergraphs) is studied in the paper. This problem arises in various applications connected with data mining in many fields. For example, in telecommunication networks maximal bicliques used for route organizing and defining subnets for marking them [3, 7]. In metabolic and genetic networks maximal bicliques are used to represent the interrelation between organisms and different external conditions [8–10]. In marketing maximal bicliques allow one to form social

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recommendations and product bundling [8–10]. Maximal bicliques are used for clustering data in various fields [11].

A new algorithm for finding all maximal induced bicliques in hypergraph is proposed in the paper. The theorem on the interrelation between induced bicliques of hypergraph and corresponding special vertex graph is proved. The theorem on time complexity and correctness of the proposed algorithm is also proved.

1. Statement of problem of finding all maximal induced bicliques of hypergraph

Let a hypergraph $H = (X, U)$ be given, where X is a finite set of vertices and U is a finite family of hyperedges of hypergraph at the same time $|X| \geqslant 1$, $|U| \geqslant 1$, and any hyperedge of hypergraph is a subset of the set X. Let us assume that $X(u)$ is a set of all vertices that incident to the hyperedge $u \in U$, and $U(x)$ is a set of all hyperedges which incident to the vertex $x \in X$. One of the ways to define hypergraph is incidence $(0,1)$-matrix I, where 1 is put in the case when hyperedge contains vertex and 0 otherwise. The degree of hyperedge $u \in U$ is the cardinality of set $|X(u)|$. Let us introduce definition that is necessary for further presentation [12].

Definition 1.1. *A hypergraph $H' = (X', U')$ is called the subhypergraph induced by the set of vertices X', where $U' = \{u' \colon X(u') = X(u) \cap X' \neq \oslash, u \in U\}$.*

Note that in Definition 1.1 $|X(u) \cap X'| \geqslant 2$ and $|u'| = 1$ for U'.

The following definition of bipartiteness of hypergraph is known, which is similar to 2-coloring. A hypergraph $H = (X, U)$ is called the bipartite when the set of vertices X can be divided into two sets S_0 and S_1 in such a way that $S_0 \cup S_1 = X$, $S_0 \cap S_1 = \oslash$ and $|X(u) \cap S_0| = 1$ is true for any hyperedge $u \in U$ [13]. To prove the main theorem, the following definition of bipartition is introduced.

Definition 1.2. *The subhypergraph $H' = (X', U')$ induced by the set of vertices X' is bipartite if there exists such partition $S_0 \cup S_1 = X'$ that $S_0 \cap S_1 = \oslash$ and $|S_0 \cap X(u')| \leqslant 1$, $|S_1 \cap X(u')| \leqslant 1$ is true for all $u' \in U'$.*

Definition 1.3. *A vertex graph of hypergraph $H = (X, U)$ is called the graph $L_2(H) = (X, E)$ which set of vertices is equal to the set of vertices X of hypergraph H while two vertices of $L_2(H)$ are adjacent if and only if corresponding vertices of hypergraph H are adjacent.*

Theorem 1.1. *The subhypergraph $H' = (X', U')$ is bipartite if and only if vertex graph $L_2(H)$ of hypergraph H contains a bipartite subgraph induced by the set of vertices X'.*

Proof. Let us prove the sufficiency. If hypergraph H contains a bipartite subgraph $H' = (X', U')$ then $L_2(H)$ contains a bipartite subgraph induced by the set X'.

The proof follows directly from Definitions 1.1–1.3. Hyperedge $u \in U$ of hypergraph H generates hyperedge u' in hypergraph H'. Then, according to Definition 1.1, the degree of hyperedge u can be greater then u', that is, $|u| \geqslant |u'|$. However, for bipartite subhypergraph $H' = (X', U')$ the degree of any hyperedge $u' \in U'$ does not exceed two. It follows from Definition 1.2. This is because if $|X(u')| > 2$ then requirement $|S_0 \cap X(u')| \leqslant 1$, $|S_1 \cap X(u')| \leqslant 1$ is violated, where $S_0 \cup S_1 = X'$ and $S_0 \cap S_1 = \oslash$. Thus, if subhypergraph $H' = (X', U')$ is bipartite then by Definition 1.3 vertex graph $L_2(H')$ is bipartite as well. On the other hand, vertex graph $L_2(H')$ is the subgraph of $L_2(H)$ induced by the set X'. Therefore, $L_2(H')$ requires bipartite subgraph of vertex graph $L_2(H)$ of hypergraph H.

Let us first prove the necessity. If vertex graph $L_2(H)$ of the hypergraph H contains the bipartite subgraph induced by the set X' then there exists the bipartite subhypergraph $H' = (X', U')$.

Let bipartite subgraph with set of vertices X' with parts S_0 and S_1 exists in graph $L_2(H)$, where $S_0 \cup S_1 = X'$, $S_0 \cap S_1 = \oslash$. Let us consider the subhypergraph $H' = (X', U')$ induced by the set X' in the hypergraph $H = (X, U)$. According to Definition 1.1, a set of hyperedges has form $U' = \{u' \colon X(u') = X(u) \cap X' \neq \oslash, u \in U\}$ in subhypergraph H'. It follows from Definition 1.3 that for any hyperedge $u \in U$ a set $X(u)$ forms a complete subgraph in the vertex graph $L_2(H)$. It is known that any bipartite graph has no complete subgraphs with number of vertices more then two [14]. Hence, any hyperedge $u' \in U'$ satisfies the inequalities $|X(u') \cap S_0| \leqslant 1$ and $|X(u') \cap S_1| \leqslant 1$ and $|u'| \leqslant 2$. □

Definition 1.4. *A bipartite graph is called the complete bipartite graph (biclique) if each vertice of one part is connected with all vertices from the second part.*

This definition can be formulated differently. If bipartite graph contains all possible edges that do not violate the bipartiteness condition then such graph is called the complete bipartite graph. A number of graph problems which belong to the class of $\sharp P$-complete or NP-complete are reduced to the search of bicliques [15]. In the general case a number of maximal bicliques depends exponentially on the size of the graph [16].

Definition 1.5. *A subhypergraph $H' = (X', U')$ induced by the set of vertices X' such that $S_0 \cup S_1 = X'$, $S_0 \cap S_1 = \oslash$ and $U' = u : s_0, s_1 \in X(u), s_0 \in S_0, s_1 \in S_1$ is called bipartite induced subhypergraph of hypergraph H.*

In what follows, by an induced bicliques of hypergraph is meant a complete bipartite induced subhypergraph of hypergraph H in the sense of Definition 1.5.

Definition 1.6. *A biclique that can not be extended with additional adjacent vertices is called the maximal induced biclique. It means that there is no another biclique which completely includes the maximal biclique.*

Definition 1.6 is true for both graphs and hypergraphs.

The problem of finding maximal biclique is well known in graph theory. There are two variants of this problem: find a maximal biclique with maximal number of vertices and find a maximal biclique with maximal number of edges. These problems arise in detection of anomalies in data, in analysing gene structures and social structures [10]. Both variants are NP-hard for general graphs [17].

Another problem associated with maximal biclique is Maximal Biclique Generation Problem (MBGP). It consists in finding all maximal bicliques for a graph. It is known that MBGP cannot be solved in polynomial time with respect to the size of input since the size of output set can be exponentially large [17]. The complexity of this problem is comparable with the complexity of problem of searching of one maximal biclique which is NP-hard [10]. The problem of maximal biclique generation can be extended to hypergraph. Such case was investigated for bihypergraphs [13].

In this paper the problem of Maximal Induced Biclique Generation Problem for Hypergraphs (MIBGP for Hypergraphs) is studied.

MIBGP for Hypergraphs. A hypergraph $H = (X, U)$ without double hyperedges is given. It is necessary to find a set of all maximal induced bicliques.

Note that problem of finding maximal induced bicliques is connected with searching of matrices of special form [18]. Let us consider interrelation between the problem of finding maximal induced bicliques and the problem of finding maximal complete submatrices of $(0,1)$-matrix.

An adjacency matrix of the vertex graph $L_2(H)$ of hypergraph H is denoted as A. Let us show the form of $(0,1)$ adjacency matrix of $L_2(H')$ for corresponding bipartite subhypergraph $H' = (X', U')$. Here S_0, S_1 are parts of hypergraph H with cardinality c and d, respectively. Since $L_2(H')$ is also the bipartite graph then adjacency matrix has form

$$A' = \begin{pmatrix} O_c & B' \\ B'^T & O_d \end{pmatrix}, \tag{1}$$

where O_c, O_d are zero matrices of sizes c and d, respectively, and B' is the matrix of size $c \times d$ which represents the adjacency of vertices between parts S_0 and S_1. Obviously, when subhypergraph H' is biclique then matrix B is a complete submatrix of matrix A. It is easy to show that any submatrix can be chosen from the set of all maximally complete submatrices in linear time with respect to the size of submatrix. Thus, in order to find induced bicliques in the hypergraph $H = (X, U)$ it is required to find such complete submatrices B' of adjacency matrix A of vertex graph $L_2(H)$ for which there is a submatrix of form (1). This is related to the problem of finding all maximally complete submatrices of the $(0,1)$-matrix.

Maximal complete submatrices can represent various combinatorial objects [19]. The problem of finding such submatrices is enumerative and belongs to the complexity class of $\sharp P$-complete problems [5, 19]. Algorithms for finding all maximal complete submatrices have high complexity with respect to the size of input matrix.

2. Algorithm of finding all maximal induced bicliques of hypergraph

Let both set of vertices and set of hyperedges of hypergraph H are lexicographically ordered.

In proposed algorithm a transition from hypergraph H to vertex graph $L_2(H)$ is considered. Adjacency matrix of $L_2(H)$ is represented as hypergraph $\Phi = (X_\Phi, U_\Phi)$. Let us introduce a definition of l-layer of hypergraph Φ with square matrix. Let us consider a subhypergraph Φ' induced by a set of vertices $S_0 \subseteq X_\Phi$ and a set of hyperedges $S_1 \subseteq U_\Phi$. If matrix of Φ' satisfy form (1) then Φ' is called induced biclique, and it is denoted by (S_0, S_1). The set of all induced bicliques (S_0, S_1) where $|S_0| = l$ is called the l-layer of hypergraph Φ.

The main idea of the algorithm involves generation of all induced bicliques for all l-layers and then choosing from them maximal induced bicliques. The HFindMIB algorithm diagram is shown in Fig. 1. Finding all maximal induced bicliques of hypergraph H is required in MIBGP for Hypergraphs. Proposed HFindMIB algorithm solves this problem in three stages. The transition from input hypergraph H to vertex graph $L_2(H)$ is realized on the initialization stage. All l-layers for adjacency matrix of vertex graph $L_2(H)$ represented as hypergraph Φ are generated on the generation stage. Finally, all maximal induced bicliques are selected from all generated l-layers n the filtration stage. This provides all maximal induced bicliques for hypergraph H. Let us shown that HFindMIB algorithm solves MIBGP for Hypergraphs correctly and estimate its time complexity. The proof of the following theorem is constructive with respect to the structure of the algorithm.

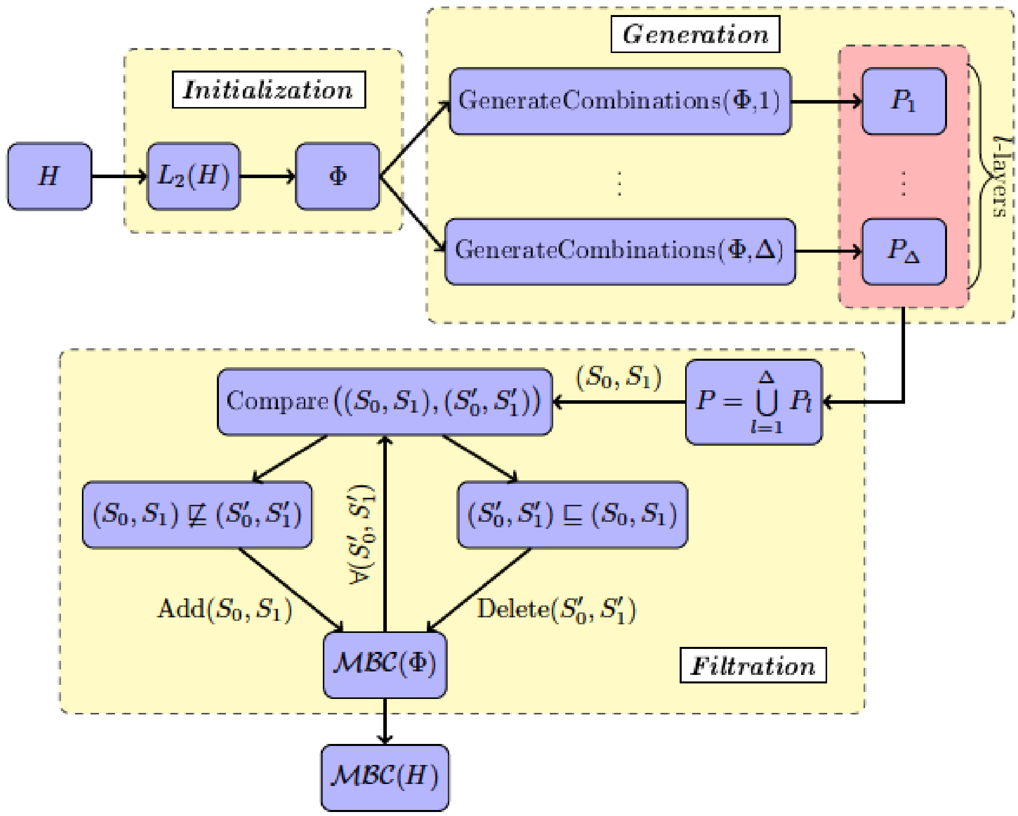

Fig. 1. Diagram of the HFindMIB algorithm

Theorem 2.1. *Let Δ be the maximum vertex degree of hypergraph $H = (X, U)$. Then HFindMIB algorithm correctly finds all maximal induced bicliques of the hypergraph, and it requires time that is not more than* $\mathcal{O}\bigg(2^{2\Delta} \cdot \Delta \cdot \big(|\mathcal{MBC}| + \Delta^3 \cdot \log(2^{2\Delta})\big) + |X|^2\bigg)$.

Proof. The HFindMIB algorithm consists of three stages. Let us consider and evaluate each stage sequentially.

Initialization stage. The HFindMIB algorithm requires a hypergraph $H = (X, U)$ with maximum vertex degree Δ as input data. The algorithm produces the vertex graph $L_2(H)$ in time $\mathcal{O}\left(|X|^2\right)$ [20]. In order to construct all induced bicliques of hypergraph H at generation phase the ability to quickly access any subset that consists of l rows in adjacency matrix of vertex graph $L_2(H)$ is needed. To achieve this artificial method is proposed. Let us fix numeration of vertices for vertex graph $L_2(H)$. Let us define a new hypergraph $\Phi = (X_\Phi, U_\Phi)$ as follows. The set of vertices X_Φ coincides up to numbering with the set of vertices of the graph $L_2(H)$. The set of hyperedges U_Φ is a system of subsets from X_Φ and it is constructed in accordance with the columns of adjacency matrix of the vertex graph $L_2(H)$. Let us note that hypergraph Φ does not allow any renumbering of vertices or hyperedges. This is necessary for one-to-one correspondence between hypergraph Φ and adjacency matrix of the vertex graph $L_2(H)$. The time requirement of the initialization stage is $\mathcal{O}(|X|^2)$.

Generation stage. Sets of all l-layers $P_l = \{(S_0, S_1) \colon S_0 \cap S_1 = \varnothing\}$, $l = 1, \ldots, \Delta$ are obtained after performing the generation stage. These sets contain all induced bicliques of the hypergraph H. Generation is carried out as follows. Sets P_l are formed for the corresponding l-layers, where $l = 1, \ldots, \Delta$. For each value of l function $GenerateCombinations(\Phi, l)$ are executed. This function generates all possible subsets $X' \subseteq X_\Phi(u)$ for each hyperedge $u \in U_\Phi$ such that $|X'| = l$ and X' satisfy (1). Form (1) ensures that all vertices of X' are not adjacent with each other. The set of all such subsets of l-layer of hyperedge $u \in U_\Phi$ is denoted as C_u^l. Each generated set X' is considered as a part S_0 of biclique. Since hypergraph Φ represents adjacency matrix of $L_2(H)$ then any $u \in U_\Phi$ can be treated as vertex of the hypergraph H. A part S_1 for corresponding set $X' \in C_u^l$ is formed from hyperedges $u \in U_\Phi$ such that they do not violate (1). If addition of u to part S_1 violates (1) then current biclique is split in two (S_0, S_1) and $(S_0, S_1 \sqcup u)$, where $S_1 \sqcup u$ is the union of elements of S_1 with u such that they are not adjacent and satisfy (1). Thus, set P_l contains all induced bicliques for which $|S_0| = l$.

Let us evaluate complexity of the generation stage. Since hypergraph $\Phi = (X_\Phi, U_\Phi)$ corresponds to the adjacency matrix of the graph $L_2(H)$ then cardinality of any $X_\Phi(u)$ does not exceed Δ, where $u \in U_\Phi$. This is because maximal degree of the vertice of hypergraph H is equal to Δ. Hence, number of all possible subsets $X' \in C_u^l$ is less than C_Δ^l. Cardinality of parts S_0, S_1 of biclique does not exceed Δ for the same reason. Therefore, the number of possible parts S_1 for any part S_0 can be estimated at 2^Δ. Obviously that this estimate much higher than the real number of possible induced bicliques because of form (1). So number of all induced bicliques for l-layer does not exceed $C_\Delta^l \cdot 2^\Delta$. For all l-layers the following estimation is true

$$2^\Delta \cdot C_\Delta^1 + \cdots + 2^\Delta \cdot C_\Delta^\Delta = 2^\Delta \cdot \left(C_\Delta^1 + \cdots + C_\Delta^\Delta\right) = 2^\Delta \cdot 2^\Delta = \mathcal{O}\left(2^{2\Delta}\right).$$

Let us note that any subset $X' \in C_u^l$ is lexicographically ordered so any X_1' and X_2' from C_u^l are comparable. This allows one to store and refresh sets P_l with tree structures like red-black tree. Subsets X_1' and X_2' can be compared in a time $\mathcal{O}(\Delta)$ because $|X'| \leqslant \Delta$. Search and addition of elements in red-black tree can be done in a time $\mathcal{O}\big(\Delta \cdot \log(2^{2\Delta})\big)$ [21]. Checking form (1) is required for split operation that can be done in a time $\mathcal{O}(\Delta^2)$ and search for adjacent vertices in part S_1 can be done in a time $\mathcal{O}(\Delta)$. So generation phase can be done in time that does not exceed $\mathcal{O}\big(2^{2\Delta} \cdot \Delta^4 \cdot \log\left(2^{2\Delta}\right)\big)$.

Filtration stage. A set of all induced bicliques P is formed from sets P_l which are l-layers of the hypergraph. It was shown that sets P_l contain all induced bicliques with parts S_0, S_1 that $|S_0| = l$ and $|S_1| \leqslant \Delta$. Union of sets P_l into set P can be done in a time $\mathcal{O}(1)$. Filtration stage cleans set P from redundant and embedded induced bicliques. Bicliques (S_0, S_1) and (S_0', S_1') where $S_0 = S_1'$ and $S_1 = S_0'$ so (S_0, S_1) and (S_0', S_1') are generated according to the specifics of generation. To find all maximal induced bicliques it is required to determine such bicliques that are embedded in others. Complexity of this process depends on the size of output set of all maximal induced bicliques $\mathcal{MBC}(\Phi)$. Comparison and detection of embedded bicliques is done in $Compare\big((S_0, S_1), (S_0', S_1')\big)$ procedure. This procedure is called for each element of P and compares it with all elements of $\mathcal{MBC}(\Phi)$. Let us define $(S_0, S_1) \sqsubseteq (S_0', S_1')$ as follows. If $S_0 \subseteq S_0', S_1 \subseteq S_1'$ or $S_1 \subseteq S_0', S_0 \subseteq S_1'$ then biclique (S_0, S_1) is embedded in (S_0', S_1'). If induced biclique $(S_0, S_1) \not\sqsubseteq (S_0', S_1')$, where $(S_0', S_1') \in P$, then it is considered as maximal and it is added into the set $\mathcal{MBC}(\Phi)$. Such operation takes $4 \cdot \Delta$ operations. It is required to filter $2^{2\Delta}$ elements of set P and compare them with the number of elements $|\mathcal{MBC}(\Phi)|$. Hence, filtration stage can be done in a time $\mathcal{O}\left(2^{2\Delta} \cdot \Delta \cdot |\mathcal{MBC}(\Phi)|\right)$ time. According to Theorem 1.1 a set $\mathcal{MBC}(\Phi)$ is equivalent to the set of all maximal induced bicliques of hypergraph H. After filtration stage only maximal induced bicliques is extracted from the set P so the HFindMIB algorithm correctly solves MIBGP for Hypergraphs.

Combining the complexity of each stage of the HFindMIB algorithm, we obtain that resulting time does not exceed

$$\mathcal{O}\Big(2^{2\Delta} \cdot \Delta \cdot \big(|\mathcal{MBC}| + \Delta^3 \cdot \log(2^{2\Delta})\big) + |X|^2\Big).$$

□

Complexity of the HFindMIB algorithm given in Theorem 2.1 depends on the size of set $\mathcal{MBC}$. This is feature of MIBGP for Hypergraphs which is an enumeration problem. Besides the estimate depends on the value of Δ. However, it is overestimated since some of the subsets at each of the l-layers does not form a part of biclique.

3. Computational experiments

To evaluate the effectiveness of solution of the MIBGP for Hypergraphs with the use of the proposed HFindMIB algorithm computational experiments were performed. Hypergraphs $H = (X, U)$ with various numbers of vertices $|X|$ and hyperedges $|U|$ and with various maximum vertex degree Δ were used in experiments. Multiple hypergraphs with the same number of vertices and with maximum degree of vertexes Δ were generated. Number of vertices of such hypergraphs was constant but number of hyperedges was varied. Computational experiments were performed on a PC with an AMD Ryzen 5 3600 6-Core Processor 3.60 GHz and 16 GB of RAM. Averaged results of experiments for generated hypergraphs are presented in Table 1.

Table 1. Results of computational experiments

Δ	$\|X\|$	$\|U\|$	$\|\mathcal{MBC}\|$	t, clocks
3	100	88,5	192	27,7
	500	438,8	965,1	446,9
	1000	870,1	1943,3	1803,2
	2500	2186,6	4845,4	12726,8
5	100	78,9	443,8	101,1
	500	371,5	2304,3	2601
	1000	732,4	4624,1	11321,1
	2500	1830	11615,9	74750,4
7	100	73,5	818,2	367,5
	500	330	4285,9	9904,3
	1000	648,3	8633,6	55452,6
	2500	1586,5	21813,7	239831

Column marked with $|U|$ represents average number of hyperedges for hypergraph with equal number of vertices and maximal degree of vertices Δ. Columns marked with $|\mathcal{MBC}|$ and t represent an average cardinality of the set of maximal induced bicliques and an average search time of the HFindMIB algorithm, respectively. The time is represented in CPU cycles. One CPU cycle time was 0,001 seconds. As can be seen from Table 1 execution time of the HFindMIB algorithm essentially depends on cardinality of set $\mathcal{MBC}$. This is typical for the problem of finding all maximal induced bicliques since their number can exponentially depend on the size of the hypergraph. Other algorithms for finding all maximal induced bicliques have similar time complexity [22, 23].

Conclusion

The problem of finding all maximal induced bicliques of hypergraph is studied in the paper. The HFindMIB algorithm for solution of this problem is proposed. The HFindMIB algorithm is based on the theorem on equivalence of induced bicliques of the hypergraph H and the vertex graph $L_2(H)$. The proof of the theorem is presented in the paper. It was shown that the proposed HFindMIB algorithm has time complexity which is not in excess of $\mathcal{O}\Big(2^{2\Delta} \cdot \Delta \cdot \big(|\mathcal{MBC}| + \Delta^3 \cdot \log(2^{2\Delta})\big) + |X|^2\Big)$, where Δ is the maximum vertex degree of hypergraph H.

The structure of the HFindMIB algorithm allows the use of parallel computing technologies to speed up the performance of the its algorithm. Refinement of the theoretical estimate of the time complexity of the algorithm is the subject for future research.

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О задаче перечисления всех максимальных индуцированных биклик гиперграфа

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Аннотация. В работе рассматривается задача поиска всех максимальных индуцированных биклик гиперграфа. Доказана теорема о связи индуцированных биклик гиперграфа H и вершинного графа $L_2(H)$. Предложен алгоритм нахождения всех максимальных индуцированных биклик. Приведена теоретическая оценка сложности предлагаемого алгоритма и доказательство его корректности. Приведены вычислительные эксперименты.

Ключевые слова: гиперграф, максимальные индуцированные биклики, алгоритм поиска.