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ON A MAXIMAL DISTANCE BETWEEN GRAPHS

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In [1], [2] some type of a metric for graphs was introduced. This type of a metric is based on the notion of maximal common subgraph (MCS). It is convenient e.g. for mathematical modelling of organic chemistry. This paper deals with the problem of a maximal distance between graphs in a given family of graphs. At the end of the paper, some problems of this theory are listed.

1. PRELIMINARIES

A graph $G = (V, E)$ consists of a non-empty finite vertex set V and edge set E. The graphs considered here are undirected without loops and multiple edges. A subgraph H of the graph G is a graph obtained from G by deleting some edges and vertices, $H \subseteq G$. Every edge $x \in E$ can be written by $x = (u, v)$, where $u, v \in V$ are vertices connected by the edge x. Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic iff there exists $1-1$ correspondence $f\colon V_1 \to V_2$ such that $(u, v) \in E_1$ if and only if $(f(u), f(v)) \in E_2$, $G_1 \cong G_2$.

A graph G is the common subgraph of the graphs G_1, G_2 iff there exist H_1, H_2 such that $H_1 \subseteq G_1$, $H_2 \subseteq G_2$ and $H_1 \cong G$, $H_2 \cong G$. A maximal common subgraph (MCS) is the common subgraph which contains the maximal number of edges.

The distance of the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is defined by

$$d(G_1, G_2) = |E_1| + |E_2| - 2|E_{1,2}| + \big|\,|V_1| - |V_2|\,\big|,$$

where $|E_1|, |E_2|, |V_1|, |V_2|$ are cardinalities of the edge sets and vertex sets respectively and $|E_{1,2}|$ is the number of edges of MCS.

Let $\mathscr{F}_{p,q}$ be the family of all graphs with p vertices and q edges. It is clear that for $G_1, G_2 \in \mathscr{F}_{p,q}$

$$d(G_1, G_2) = 2q - 2|E_{1,2}|\,.$$

If we identify the isomorphic graphs then $\mathscr{F}_{p,q}$ with the distance d is a metric space.

Without loss of generality we can suppose that all graphs in $\mathscr{F}_{p,q}$ have the same vertex set V.

2. DIAMETER OF A FAMILY OF GRAPHS

We define

$$\operatorname{diam} \mathscr{F}_{p,q} = \max \{d(G, H);\ G, H \in \mathscr{F}_{p,q}\}.$$

Evidently, $\operatorname{diam} \mathscr{F}_{p,0} = \operatorname{diam} \mathscr{F}_{p,1} = 0$. We shall try to find out or to estimate $\operatorname{diam} \mathscr{F}_{p,q}$ for arbitrary p, q. We remark that

$$0 \leqq q \leqq \binom{p}{2}.$$

Theorem 1. *Let $G_1, G_2 \in \mathscr{F}_{p,q}$, where $q \geqq 1$. Then*

$$d(G_1, G_2) \leqq 2q - 2.$$

Proof. MCS of the graphs G_1 and G_2 contains at least one edge.

The consequence of this theorem is: $\operatorname{diam} \mathscr{F}_{p,q} \leqq 2q - 2$.

Theorem 2. *Let $q \geqq 1$. Then* $\operatorname{diam} \mathscr{F}_{p,q} = 2q - 2$ *iff* $q \leqq \frac{1}{2}p$.

Proof. Let $q \leqq \frac{1}{2}p$ and $V = \{v_1, v_2, \ldots, v_p\}$. We construct $G_1 = (V, E_1)$, $G_2 = (V, E_2)$, where

$$E_1 = \{(v_1, v_2), (v_1, v_3), \ldots, (v_1, v_{q+1})\},$$
$$E_2 = \{(v_1, v_2), (v_3, v_4), \ldots, (v_{2q-1}v_{2q})\}.$$

MCS of of these graphs consist of one edge only. Therefore $d(G_1, G_2) = 2q - 2$. Using Theorem 1 we have $\operatorname{diam} \mathscr{F}_{p,q} = 2q - 2$. Conversely, let $\operatorname{diam} \mathscr{F}_{p,q} = 2q - 2$ and let $q > \frac{1}{2}p$. Then for any $G_1, G_2 \in \mathscr{F}_{p,q}$ we have $\sum \deg v_i = 2q > p$, where $\deg v_i$ is number of edges incident with the vertex v_i. It implies the existence of vertices u, v such that $\deg u \geqq 2$ in G_1 and $\deg v \geqq 2$ in G_2. Then MCS of the graphs G_1, G_2 contains at least two edges. Therefore $d(G_1, G_2) \leqq 2q - 4$ for any $G_1, G_2 \in \mathscr{F}_{p,q}$. It contradicts the assumption.

Theorem 3. *Let $\frac{1}{2}p < q \leqq p - 1$. Then* $\operatorname{diam} \mathscr{F}_{p,q} = 2q - 4$.

Proof. Theorem 2 implies that $\operatorname{diam} \mathscr{F}_{p,q} < 2q - 2$. We construct $G_1 = (V, E_1)$, $G_2 = (V, E_2)$ such that

$$E_1 = \{(v_1, v_2), (v_1, v_3), \ldots, (v_1, v_{q+1})\},$$
$$E_2 = \{(v_1, v_2), (v_2, v_3), \ldots, (v_q, v_{q+1})\}.$$

Then $G_1, G_2 \in \mathscr{F}_{p,q}$ and their MCS contains two edges only. Therefore $d(G_1, G_2) = 2q - 4$. It implies $2q - 4 \leqq \operatorname{diam} \mathscr{F}_{p,q}$. It proves that $\operatorname{diam} \mathscr{F}_{p,q} = 2q - 4$.

A complement of the graph $G = (V, E)$ is a graph $\bar{G} = (V, \bar{E})$ which contains just the edges which don't belong to E. It is clear that $|E| + |\bar{E}| = \frac{1}{2}p(p - 1)$. In [3], it was proved:

Theorem 4. *For arbitrary graphs G, H with the same number of vertices the following holds*: $d(G, H) = d(\bar{G}, \bar{H})$.

Theorem 5. *If we denote* $\bar{q} = \frac{1}{2}p(p-1) - q$ *then*

$$\operatorname{diam} \mathscr{F}_{p,q} = \operatorname{diam} \mathscr{F}_{p,\bar{q}}$$

Theorem 6. *Let* $q \geqq \frac{1}{2}p(p-2)$. *Then*

$$\operatorname{diam} \mathscr{F}_{p,q} = p(p-1) - 2q - 2\,.$$

Proof. If $q \geqq \frac{1}{2}p(p-2)$ then

$$\bar{q} = \frac{p}{2}(p-1) - q \leqq \frac{p}{2}(p-1) - \frac{p}{2}(p-2) = \frac{p}{2}.$$

Using Theorem 2 and Theorem 5 we get

$$\operatorname{diam} \mathscr{F}_{p,q} = \operatorname{diam} \mathscr{F}_{p,\bar{q}} = 2\bar{q} - 2 = p(p-1) - 2q - 2\,.$$

Theorem 7. Let

$$\binom{p-1}{2} \leqq q < \frac{p}{2}(p-2)\,.$$

Then

$$\operatorname{diam} \mathscr{F}_{p,q} = p(p-1) - 2q - 4\,.$$

Proof. The inequality

$$\binom{p-1}{2} \leqq q < \frac{p}{2}(p-2)$$

follows $\frac{1}{2}p < \bar{q} \leqq p - 1$. Then

$$\operatorname{diam} \mathscr{F}_{p,q} = \operatorname{diam} \mathscr{F}_{p,\bar{q}} = 2\bar{q} - 4 = p(p-1) - 2q - 4\,.$$

PROBLEMS

It would be interesting to solve some problems connected with the notion of distance and diameter. We found out

$$\operatorname{diam} \mathscr{F}_{p,q} \quad \text{for} \quad q \leqq p - 1 \quad \text{or} \quad q \geqq \binom{p-1}{2}.$$

It implies that we know all $\operatorname{diam} \mathscr{F}_{p,q}$ for $p \leqq 4$.

Problem 1. How to find out or estimate $\operatorname{diam} \mathscr{F}_{p,q}$ for

$$4 < p \leqq q < \binom{p-1}{2}?$$

The next problems are connected with the problems of distance between graphs with the sanme number of vertices and different number of edges.

Problem 2. If $G_1 \in \mathscr{F}_{p,q}$, $G_2 \in \mathscr{F}_{p,q_2}$, $q_1, q_2 \geqq 1$ then

$$d(G_1, G_2) \leqq q_1 + q_2 - 2\,.$$

Under which conditions the equality holds?

Problem 3. Obviously,

$$\operatorname{diam}(\mathscr{F}_{p,q_1} \cup \mathscr{F}_{p,q_2}) \geqq \max(\operatorname{diam} \mathscr{F}_{p,q_1}, \operatorname{diam} \mathscr{F}_{p,q_2}).$$

For which p, q_1, q_2

a) $\operatorname{diam}(\mathscr{F}_{p,q_1} \cup \mathscr{F}_{p,q_2}) > \max(\operatorname{diam} \mathscr{F}_{p,q_1}, \operatorname{diam} \mathscr{F}_{p,q_2})$,

b) $\operatorname{diam}(\mathscr{F}_{p,q_1} \cup \mathscr{F}_{p,q_2}) = \max(\operatorname{diam} \mathscr{F}_{p,q_1}, \operatorname{diam} \mathscr{F}_{p,q_2})$?

Problem 4. Is any relation between $\operatorname{diam}(\mathscr{F}_{p,q_1} \cup \mathscr{F}_{p,q_2})$ and $\operatorname{diam} \mathscr{F}_{p,q_1} + \operatorname{diam} \mathscr{F}_{p,q_2}$? Are there any non-trivial p, q_1, q_2 such that these numbers are the same?

Problem 5. Prove or reject the conjecture: If

$$q_1 \leqq q_2 \leqq \frac{1}{2} \frac{p}{2}(p - 1)$$

then $\operatorname{diam} \mathscr{F}_{p,q_1} \leqq \operatorname{diam} \mathscr{F}_{p,q_2}$.

The last problem deals with the distance of graphs which have different numbers of vertices and edges. It is clear

$$d(G_1, G_2) \leqq q_1 + q_2 + |p_1 - p_2| - 2$$

for $G_1 \in \mathscr{F}_{p_1,q_1}$, $G_2 \in \mathscr{F}_{p_2,q_2}$, $q_1, q_2 \geqq 1$.

Problem 6. Under which conditions

a) $d(G_1, G_2) = q_1 + q_2 + |p_1 - p_2| - 2$,

b) $d(G_1, G_2) = q_1 + q_2 + |p_1 - p_2| - 4$ hold?

Remark. B. Zelinka [4] solved the problem of $\operatorname{diam} \mathscr{F}_p$, where $\mathscr{F}_p = \bigcup_q \mathscr{F}_{p,q}$ is the family of all graphs with p vertices. He proved that $\operatorname{diam} \mathscr{F}_p = \frac{1}{2}p(p - 1)$.

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