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Comparing variable Zagreb indices

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Abstract

The first and second Zagreb indices are defined as $M_1 = \sum_{i \in V} d_i^2$ and $M_2 = \sum_{(i,j) \in E} d_i d_j$. Recently, it has been proved that $M_1 / n \le M_2 / m$ (where m is the number of edges and n the number of vertices) for chemical graphs and that this result does not hold for general graphs. Here, generalizations of this result are analyzed. Variable first and second Zagreb indices are defined by ${}^{\lambda}M_1 = \sum_{i \in V} d_i^{2\lambda}$ and ${}^{\lambda}M_2 = \sum_{(i,j) \in E} d_i^{\lambda} d_j^{\lambda}$. In this paper, it is shown that ${}^{\lambda}M_1 / n \le {}^{\lambda}M_2 / m$ for all graphs and for all $\lambda \in [0, 1/2]$; and that ${}^{\lambda}M_1 / n \le {}^{\lambda}M_2 / m$ for all chemical graphs for all $\lambda \in [0,1]$. Also, it is shown that for every $\lambda \in R \setminus [0,1]$ and every complete unbalanced bipartite graphs G it holds that ${}^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m$. Hence, the results for chemical graphs cannot be extended. It is shown that for each $\lambda \in R \setminus \left[0, \sqrt{2}/2\right]$, there is graph G such that ${}^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m$. As an open problem remains the question if ${}^{\lambda}M_1 / n \le {}^{\lambda}M_2 / m$ holds for all graphs for some $\lambda \in \left(1/2, \sqrt{2}/2\right]$.

Introduction

The first and second Zagreb indices are among the oldest and the most famous topological indices (see [1-4] and references within) and they are defined as:

$$M_1 = \sum_{i \in V} d_i^2 \text{ and } M_2 = \sum_{(i,j) \in E} d_i d_j ,$$

where V is the set of vertices, E is set of edges and d_i is degree of vertex i.

These indices have been generalized to variable first and second Zagreb indices [5] defined as

$$M_1 = \sum_{i \in V} d_i^{2\lambda} \text{ and } M_2 = \sum_{(i,j) \in E} \left(d_i d_j\right)^{\lambda}.$$

Recently, the system AutoGraphiX [6-8] proposed the following conjecture:

Conjecture 1. For all simple connected graphs G,

$$M_1 / n \leq M_2 / m$$

and the bound is tight for complete graphs.□

In the paper [9], it has been shown that this conjecture is not true. However, the claim holds if we restrict our attention to the class of chemical graphs (i.e., graphs with maximal degree at most 4). Namely, the following theorem is given [9]:

Theorem 1. For all chemical graphs G with order n, size m, first and second Zagreb indices M_1 and M_2,

$$M_1 / n \leq M_2 / m.$$

Moreover, the bound is tight if and only if all edges (i, j) have the same pair (d_i, d_j) of degrees or if the graph is composed of disjoint stars S_5 and cylces $C_p, C_q, \ldots$ of any length.□

The aim of this paper is to analyze the generalization of this problem to variable Zagreb indices. It will be shown that the claim analogous to the proposed conjecture holds for all $\lambda \in [0, 1/2]$, namely that:

Theorem 2. For all graphs G and all $\lambda \in [0, 1/2]$, it holds that ${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m$.□

The analogue of Theorem 1 can be proved for $\lambda \in [0, 1]$, i.e., it will be proved that:

Theorem 3. For all chemical graphs G and all $\lambda \in [0, 1]$, it holds that ${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m$.□

In order to see that the results of Theorem 3 cannot be extended, it will be proved that:

Theorem 4. Let $\lambda \in R \setminus [0, 1]$ and G be any complete unbalanced bipartite graph. Then, ${}^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m$.□

It remains to analyze possible extensions of Theorem 2. In [9], it is shown that there is graph G such that ${}^{1}M_1(G)/n > {}^{1}M_2(G)/m$. Hence, it remains to analyze the interval $(1/2,1)$. It will be proved that

Theorem 5. Let $\lambda \in \left(\sqrt{2}/2,1\right)$. Then, there is a graph G such that ${}^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m$.□

The remaining open problem is:

Open problem: Identify $\lambda \in \left(1/2,\sqrt{2}/2\right]$ such that ${}^{\lambda}M_1/n > {}^{\lambda}M_2/m$ for all graphs G.

Main results

We start with an arbitrary Lemma:

Lemma 1. Let i and j be different natural numbers and let

$$f(i,j) = i^{\lambda} \cdot j^{\lambda} \cdot \left(\frac{1}{i} + \frac{1}{j}\right) - i^{2\lambda-1} - j^{2\lambda-1}.$$

Then, $f(i,j) \geq 0$ for $\lambda \in [0,1]$ and $f(i,j) < 0$ for $\lambda \in R \setminus [0,1]$.

Proof: Note that the expression above is symmetric in i and j. Hence, we may assume that $i > j$. Denote $x = \frac{i}{j} > 1$. We have:

$$\begin{aligned}
& i \cdot j \cdot f(i,j) = i^{\lambda} \cdot j^{\lambda} \cdot (i+j) - i^{2\lambda} \cdot j - i \cdot j^{2\lambda} \\
& \frac{i \cdot j \cdot f(i,j)}{j^{2\lambda-1}} = x^{\lambda+1} + x^{\lambda} - x^{2\lambda} - x \\
& \frac{i \cdot j \cdot f(i,j)}{j^{2\lambda-1}} = x \cdot \left(1 - x^{\lambda-1}\right) \cdot \left(x^{\lambda} - 1\right).
\end{aligned}$$

Hence, $f(i,j)$ has the same sign as $x \cdot \left(1 - x^{\lambda-1}\right) \cdot \left(x^{\lambda} - 1\right)$. Note that

$$x > 0 \text{ and } \left\{ \begin{array}{ll} 1 - x^{\lambda-1} \geq 0, & \text{for each } \lambda \leq 1 \\ 1 - x^{\lambda-1} < 0, & \text{for each } \lambda > 1 \end{array} \right\} \text{ and } \left\{ \begin{array}{ll} x^{\lambda} - 1 \geq 0, & \text{for each } \lambda \geq 0 \\ x^{\lambda} - 1 < 0, & \text{for each } \lambda < 0 \end{array} \right\}.$$

Hence,

$$\begin{array}{ll} x \cdot \left(1 - x^{\lambda-1}\right) \cdot \left(x^{\lambda} - 1\right) \geq 0, & \text{for each } \lambda \in [0,1] \\ x \cdot \left(1 - x^{\lambda-1}\right) \cdot \left(x^{\lambda} - 1\right) < 0, & \text{for each } \lambda \in R \setminus [0,1] \end{array},$$

which proves the Lemma. ■

Now, theorem 2 can be proved.

Proof of Theorem 2: Denote by m_{ij} the number of edges with end-vertices i and j. We have:

$$\frac{M_1(G)}{n} = \frac{\sum_{v\in V(G)} d(v)^{2\lambda}}{\sum_{i\in N} n_i} = \frac{\sum_{i\in N} n_i \cdot i^{2\lambda}}{\sum_{i\in N} \frac{m_{ii} + \sum_{j\in N} m_{ij}}{i}} = \frac{\sum_{i\in N}\left(\frac{m_{ii} + \sum_{j\in N} m_{ij}}{i} \cdot i^{2\lambda}\right)}{\sum_{i\le j} m_{ij} \cdot \left(\frac{1}{i} + \frac{1}{j}\right)}$$

$$= \frac{\sum_{i\in N}\left(\left(m_{ii} + \sum_{j\in N} m_{ij}\right) \cdot i^{2\lambda-1}\right)}{\sum_{i\le j} m_{ij} \cdot \left(\frac{1}{i} + \frac{1}{j}\right)} = \frac{\sum_{i\le j} m_{ij} \cdot \left(i^{2\lambda-1} + j^{2\lambda-1}\right)}{\sum_{i\le j} m_{ij} \cdot \left(\frac{1}{i} + \frac{1}{j}\right)}$$

and

$$\frac{M_2(G)}{m} = \frac{\sum_{uv\in E(G)} d(u)\cdot d(v)}{m} = \frac{\sum_{i\le j\in N} m_{ij} \cdot i^{\lambda} \cdot j^{\lambda}}{\sum_{i\le j\in N} m_{ij}}.$$

Hence, we need to prove that:

$$\frac{\sum_{i\le j} m_{ij} \cdot \left(i^{2\lambda-1} + j^{2\lambda-1}\right)}{\sum_{k\le l} m_{kl} \cdot \left(\frac{1}{k} + \frac{1}{l}\right)} \le \frac{\sum_{i\le j\in N} m_{ij} \cdot i^{\lambda} \cdot j^{\lambda}}{\sum_{k\le l\in N} m_{kl}}$$

$$\left[\sum_{i\le j\in N} m_{ij} \cdot i^{\lambda} \cdot j^{\lambda}\right] \cdot \left[\sum_{k\le l} m_{kl} \cdot \left(\frac{1}{k} + \frac{1}{l}\right)\right] - \left[\sum_{i\le j} m_{ij} \cdot \left(i^{2\lambda-1} + j^{2\lambda-1}\right)\right] \cdot \left[\sum_{k\le l\in N} m_{kl}\right] \ge 0$$

$$\sum_{\substack{i\le j \\ k\le l \\ i,j,k,l\in N}} \left[\left(i^{\lambda} \cdot j^{\lambda} \cdot \left(\frac{1}{k} + \frac{1}{l}\right) - i^{2\lambda-1} - j^{2\lambda-1}\right) \cdot m_{ij} \cdot m_{kl}\right] \ge 0.$$

Now, collecting in the same summand cases where roles of (i, j) and (k,l) are reversed one gets:

$$\sum_{\substack{i\le j\\ i,j\in N}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}\right)\cdot m_{ij}^{\ 2}\right]+$$
$$\sum_{\substack{i\le j\\ k\le l\\ \{(i,j),(k,l)\}\subseteq N^2\\ (i,j)\ne(k,l)}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}\right)\cdot m_{ij}\cdot m_{kl}\right]\ge 0. \tag{1}$$

From Lemma 1, it follows that all the summands in the first sum are non-negative. Hence, it is sufficient to prove that all the summands in the second sum are also non-negative, i.e., that for each i, j, k and l it holds:

$$g(i,j,k,l)=i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}.$$

Without loss of generality, we may assume that $i=\max\{i,j,k,l\}$ and that $k\ge l$.

$$\frac{\partial g(i,j,k,l)}{\partial i}=\frac{\lambda\cdot i^{\lambda-1}\cdot j^{\lambda}}{k}+\frac{\lambda\cdot i^{\lambda-1}\cdot j^{\lambda}}{l}-\frac{1}{i^2}\cdot k^{\lambda}\cdot l^{\lambda}-(2\lambda-1)\cdot i^{2\lambda-2}=$$
$$=\lambda\cdot\frac{i^{\lambda}\cdot j^{\lambda}}{k\cdot i}+\lambda\cdot\frac{i^{\lambda}\cdot j^{\lambda}}{l\cdot i}+(1-2\lambda)\cdot\frac{i^{2\lambda}}{i^2}-\frac{k^{\lambda}\cdot l^{\lambda}}{i^2}$$

Since, $\frac{i^{\lambda}\cdot j^{\lambda}}{k\cdot i},\frac{i^{\lambda}\cdot j^{\lambda}}{l\cdot i},\frac{i^{2\lambda}}{i^2}\ge\frac{k^{\lambda}\cdot l^{\lambda}}{i^2}$, it follows that $\frac{\partial g(i,j,k,l)}{\partial i}\ge 0$. Hence, it is sufficient to prove the claim when $i=\max\{j,k,l\}$. Distinguish two cases:

CASE 1: $i=j$.

In this case $i^{\lambda}\cdot j^{\lambda}\ge k^{\lambda}\cdot l^{\lambda}$ and $\frac{1}{k}+\frac{1}{l}\ge\frac{1}{i}+\frac{1}{j}$, hence

$$g(i,j,k,l)\ge i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}=$$
$$=\left[i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}\right]+\left[k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)-k^{2\lambda-1}-l^{2\lambda-1}\right]\ge\{\text{from Lemma 1}\}\ge 0,$$

which proves the claim.

CASE 1: $i=k$.

Without loss of generality, we may assume that $j\ge l$. Note that

$$\frac{g(i,j,i,l)}{\partial l}=-\frac{i^{\lambda}\cdot j^{\lambda}}{l^2}+\lambda\cdot\frac{i^{\lambda}\cdot l^{\lambda}}{i\cdot l}+\lambda\cdot\frac{i^{\lambda}\cdot l^{\lambda}}{j\cdot l}+(1-2\lambda)\cdot\frac{l^{2l}}{l^2}.$$

Since, $\frac{i^{\lambda}\cdot j^{\lambda}}{l^2}\geq\frac{i^{\lambda}\cdot l^{\lambda}}{i\cdot l},\frac{i^{\lambda}\cdot l^{\lambda}}{j\cdot l},\frac{l^{2l}}{l^2}$ it follows that $\frac{\partial g(i,j,k,l)}{\partial i}\leq 0$. Hence, it is sufficient to prove the claim when $l=j$. We have:

$$g(i,j,i,j)=i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)+i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-i^{2\lambda-1}-j^{2\lambda-1},$$

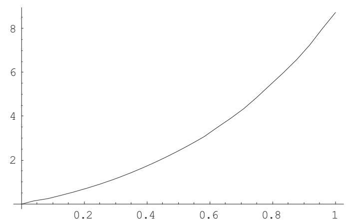
and the claim follows from Lemma 1.■

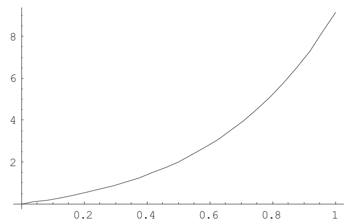
Let us prove Theorem 3:

Proof of Theorem 3: Similarly as in the proof of Theorem 2, one obtains that it is sufficient to prove that:

$$\sum_{\substack{i\leq j\\ i,j\in N}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}\right)\cdot {m_{ij}}^{2}\right]+$$
$$\sum_{\substack{i\leq j\\ k\leq l\\ \{(i,j),(k,l)\}\subseteq N^2\\ (i,j)\neq(k,l)}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}\right)\cdot m_{ij}\cdot m_{kl}\right]\geq 0.$$

From Lemma 1, it follows that all the summands in the first sum are non-negative. Hence, it is sufficient to prove that all the summands in the second sum are also non-negative. Since, the maximum degree is at most 4, there are 45 summands. Graphs of all 45 functions $f_{(i,j),(k,l)}:[0,1]\rightarrow R$ are drawn using the software package *Mathematica* [10]. Here, we present just 6 of them:





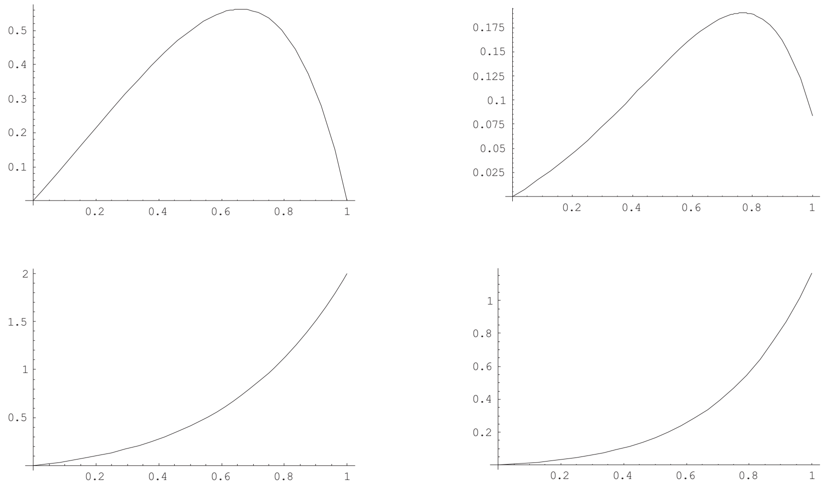


Figure 1. Graphs of the functions $f_{(1,1),(2,4)}$, $f_{(1,2),(3,4)}$, $f_{(1,4),(2,2)}$, $f_{(2,4),(3,3)}$, $f_{(2,4),(4,4)}$ and $f_{(3,3),(4,4)}$.

From these 45 graphs the claim easily follows. ■

Let us prove Theorem 4:

Proof of Theorem 4: Denote by a and b the cardinalities of the classes of bipartition. Obviously all m_{ij} s are equal to 0 except m_{ab}. Along the same lines as in the proof of Theorem 3 (just with the reversed inequality sign) one gets that it is sufficient to prove that:

$$\left(a^{\lambda}\cdot b^{\lambda}\cdot\left(\frac{1}{a}+\frac{1}{b}\right)-a^{2\lambda-1}-b^{2\lambda-1}\right)\cdot m_{ab}<0\,.$$

Obviously $m_{ab}>0$ and the from Lemma 1, it follows that $a^{\lambda}\cdot b^{\lambda}\cdot\left(\frac{1}{a}+\frac{1}{b}\right)-a^{2\lambda-1}-b^{2\lambda-1}<0$.■

Before proving Theorem 5, we prove another two more Lemmas:

Lemma 2. For each $\lambda\in\left(\sqrt{2}/2,1\right)$, there are rational numbers $a,b<1$ such that:

$$\begin{aligned}&\lambda+a\lambda-b<2\lambda-1\\&2b\lambda-1<2\lambda-1\\&2b\lambda-a<2\lambda-1.\end{aligned}$$

Proof: It we take $1/2$ for a and $\frac{1}{\sqrt{2}}+1-\sqrt{2}$ for b all three inequalities will be satisfied. Since the set of rational numbers is dense in R; all functions continuous; and all inequalities sharp, it follows that the inequalities are also satisfied for some rational numbers a and b. ■

Lemma 3. For each $\lambda \in \left(\sqrt{2}/2,1\right)$, there are integers $i,j,k,l>1$ such that $k=l$ and:

$$g\left(i,j,k,l\right)=i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}<0$$

Proof: Let a and b be rational numbers that satisfy the conditions of the last Lemma and let r be the common denominator of a and b. Denote $a=\frac{p}{r}$ and $b=\frac{q}{r}$. Let x be any integer. Note that:

$$g\left(x^{r},x^{p},x^{q},x^{q}\right)=x^{r\lambda+p\lambda-q}+x^{r\lambda+p\lambda-q}+x^{2q\lambda-p}+x^{2q\lambda-r}-x^{r\cdot(2\lambda-1)}-x^{p\cdot(2\lambda-1)}-x^{q\cdot(2\lambda-1)}-x^{q\cdot(2\lambda-1)}=$$
$$=2\cdot\left(x^{r}\right)^{\lambda+a\lambda-b}+\left(x^{r}\right)^{2b\lambda-a}+\left(x^{r}\right)^{2b\lambda-1}-\left(x^{r}\right)^{(2\lambda-1)}-\left(x^{r}\right)^{a\cdot(2\lambda-1)}-2\cdot\left(x^{r}\right)^{b\cdot(2\lambda-1)}$$

If x goes to infinity, the sign will be determined by the coefficient standing with the largest exponent and that is (from the last Lemma) $2\lambda-1$. Hence, indeed the claim holds. ■

Now, we can prove Theorem 5.

Proof of Theorem 5: We need to show that there is graph G such that

$$\sum_{\substack{i\le j\\ i,j\in N}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}\right)\cdot m_{ij}{}^{2}\right]+$$
$$\sum_{\substack{i\le j\\ k\le l\\ \{(i,j),(k,l)\}\subseteq N^2\\ (i,j)\neq(k,l)}}\left[\left(i^{\lambda}\cdot j^{\lambda}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)+k^{\lambda}\cdot l^{\lambda}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)-i^{2\lambda-1}-j^{2\lambda-1}-k^{2\lambda-1}-l^{2\lambda-1}\right)\cdot m_{ij}\cdot m_{kl}\right]<0,$$

i.e., that:

$$\sum_{\substack{i\le j\\ i,j\in N}}\left[\frac{1}{2}g\left(i,j,i,j\right)\cdot m_{ij}{}^{2}\right]+\sum_{\substack{i\le j\\ k\le l\\ \{(i,j),(k,l)\}\subseteq N^2\\ (i,j)\neq(k,l)}}\left[g\left(i,j,k,l\right)\cdot m_{ij}\cdot m_{kl}\right]<0,$$

Let i,j,k (and $l=k$) be taken in such way that satisfy the conditions of the last Lemma. Let $G_{x,y}$ be graph created in the following way:

1) Take x copies of K_{ij} (complete bipartite graph with i vertices in one class and j in other class) and y copies of K_{kk}.
2) Connect each of these graphs (cyclically) with two neighboring graphs and delete in each graph one edge in order not to change degrees (see figure below; the edges that should be deleted are drawn with dashed lines and edges that should be added by solid lines)

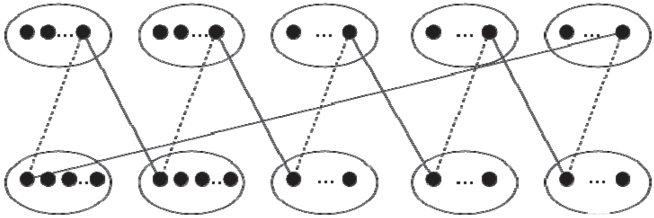


Figure 2. Graph G_{xy}.

We have: $m_{ij} = m_{ji} = xij - 1$, $m_{kk} = yk^2 - 1$, $m_{ik} = m_{ki} = 1$, $m_{jk} = m_{kj} = 1$ and all other m s are equal to 0. Hence, we need to prove that for some x and y we have:

$$\begin{aligned}
&\frac{1}{2} g(i,j,i,j) \cdot (ijx-1)^2 + g(i,j,k,k) \cdot (k^2 y - 1) \cdot (ijx-1) + g(i,j,i,k) \cdot (ijx-1) \\
&+ g(i,j,j,k) \cdot (ijx-1) + \frac{1}{2} g(k,k,k,k) \cdot (k^2 y-1)^2 + g(k,k,i,k) \cdot (k^2 y - 1) + \qquad (2) \\
&g(k,k,j,k) \cdot (k^2 y-1) + \frac{1}{2} g(i,k,i,k) + g(i,k,j,k) + \frac{1}{2} g(j,k,j,k) < 0
\end{aligned}$$

Putting $y = x^2$ we get that the coefficient standing by x^4 is $g(k,k,k,k) = 0$ and the coefficient standing by x^3 is $g(i,j,k,k) \cdot k^2 \cdot ij$ which is a negative number. Hence for sufficiently large x, relation (2) will hold. ■

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