CONJECTURE FOR THE GEOMETRIC-ARITHMETIC INDEX WITH GIVEN MINIMUM DEGREE

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Beograd, 2016

Introduction to the Geometric-Arithmetic index

- **Abstract.** The geometric-arithmetic index $GA(G)$ of a graph is defined as sum of weights of all edges of graph. The weight of one edge is quotient of the geometric and arithmetic mean of degrees of its end vertices $\frac{2\sqrt{d_u d_v}}{d_u+d_v}$. The predictive power of GA for physico-chemical properties is somewhat better than the predictive power of other connectivity indices. Let $G(k,n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k. We give a conjecture about lower bounds and structure of extremal graphs of this index for n-vertex graphs with given minimum degree k.

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- *Keywords*: Geometric-arithmetic index, Linear programming.

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- The Geometric-Arithmetic is:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

where the summation goes over all edges uv of G.

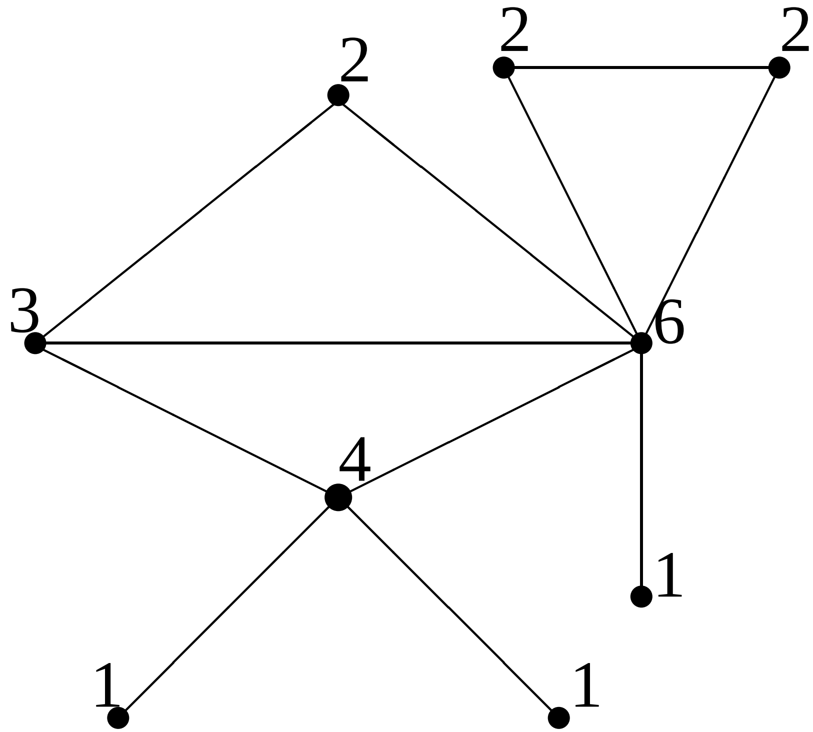

Fig. 1. $$GA(G) = 2\frac{2\sqrt{1\cdot 4}}{5} + \frac{2\sqrt{1\cdot 6}}{7} + \frac{2\sqrt{2\cdot 2}}{4} + \frac{2\sqrt{2\cdot 3}}{5} + 3\frac{2\sqrt{2\cdot 6}}{8} + \frac{2\sqrt{3\cdot 4}}{7} + \frac{2\sqrt{3\cdot 6}}{9} + \frac{2\sqrt{4\cdot 6}}{10}$$

Introduction to the Geometric-Arithmetic index

- In fact, this index belongs to wider class of so-called *geometric-arithmetic general* topological indices. A class of geometric-arithmetic general topological indices is defined in [9]

$$GA_{general}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v},$$

where Q_u is some quantity that (in a unique manner) can be associated with the vertex u of the graph G.

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Introduction to the Geometric-Arithmetic index

- The second member of this class was considered by Fath-Tabar et al. [9] by setting Q_u to be the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}.$$

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- Zhou et al. [19] proposed a third member of the class of $GA_{general}$ by setting Q_u to be the number m_u of the edges of G, lying closer to vertex u than to vertex v.

Known results for the Geometric-Arithmetic index

- It is noted in [17] that the predictive power of GA for physico-chemical properties (boiling point, entropy, enthalpy and standard enthalpy of vaporisation, enthalpy of formation, acentric factor) is somewhat better than the predictive power of the Randić connectivity index.

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- In [18] Yuan, Yhou and Trinajsić gave the lower and upper bounds for GA index of molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the first, second and third minimum and maximum GA indices.

Known results for the Geometric-Arithmetic index

- The Randić connectivity index was studied by chemists and mathematicians and there are a lot of papers about it. Several books are devoted to the Randić index. Recently, the geometric-arithmetic index attracted attention of mathematicians also, but there are few papers about it, dedicated to molecular graphs ([8], [12]).

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- In [5],K. Das, I. Gutman, B. Furtula, *Survey on Geometric - Arithmetic Indices of Graphs*, MATCH-Communications in Mathematical and in Computer Chemistry, 65 (2011), 595-644, authors are collected all obtained results on class GA indices.

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- In [6] T. Divnić, M. Milivojević, Lj. Pavlović, *Extremal graphs for the geometric-arithmetic index with given minimum degree*, Discrete Applied Mathematics, Vol. 162, 2014, 386-390, authors found extremal graphs for GA index for some given minimum degree.

Conjecture about the extremal graphs

- Denote by $f_t(k) = \frac{(n-t)(k-t)}{2} + \frac{2\sqrt{k(n-t)}}{k+n-t} t(n-t)$ for $0 \le t \le k$, $k \le k_0$ and by $k_t \in [0, k_0]$ a unique root of equation $f_{t+1} - f_t = 0$.

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- **Conjecture.** *If G is a connected simple n vertex graphs with minimum vertex degree k, then*

Conjecture about the extremal graph

- $GA \geq$

$$
\begin{cases}
\frac{kn}{2}, & \lceil k_0 \rceil \leq k \\
\frac{(n-1)(k-1)}{2} + \frac{2\sqrt{k(n-1)}}{k+n-1}(n-1), & \lceil k_1 \rceil \leq k \leq \lfloor k_0 \rfloor, \\
\frac{(n-2)(k-2)}{2} + \frac{2\sqrt{k(n-2)}}{k+n-2}2(n-2), & \lceil k_2 \rceil \leq k \leq \lfloor k_1 \rfloor, \\
\frac{(n-3)(k-3)}{2} + \frac{2\sqrt{k(n-3)}}{k+n-3}3(n-3), & \lceil k_3 \rceil \leq k \leq \lfloor k_2 \rfloor, \\
\vdots & \vdots \\
\frac{(n-t)(k-t)}{2} + \frac{2\sqrt{k(n-t)}}{k+n-t}t(n-t), & \lceil k_t \rceil \leq k \leq \lfloor k_{t-1} \rfloor, \\
\vdots & \vdots \\
\frac{2\sqrt{k(n-k)}}{k+n-k}k(n-k), & k \leq \lfloor k_{k-1} \rfloor.
\end{cases}
$$

Conjecture about the extremal graphs

- **Remark.** *If* $\lceil k_t(n)\rceil \le k \le \lfloor k_{t-1}(n)\rfloor$ *and* $(n-t)(k-t)$ *is even, the lower bound is attained on graphs* $G_{k,n-t}$ *which have* $n_k = n-t,\ n_{n-t} = t,\ x_{k,n-t} = t(n-t)$, $x_{k,k} = \frac{(n-t)(k-t)}{2}$ *and all other* $x_{ij} = 0.$

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- *Extremal graph* $G_{k,n-t}$ *is complete join* $G_1 + G_2$ *of graphs* G_1 *and* G_2. G_1 *is regular graph on* $n-t$ *vertices with degree* $k-t$ *and* G_2 *is graph on* t *isolated vertices (with degree 0). The complete join of two graphs is their graph union with all the edges that connect the vertices of the first graph with the vertices of the second graph.*

A quadratic programming model of the problem

- $$\min\ GA(G) = \sum_{\substack{k\le i\le n-1\\ i\le j\le n-1}} \frac{2\sqrt{ij}}{i+j} x_{i,j}$$

$$\begin{array}{ccccccccc}
2x_{k,k} & + & x_{k,k+1} & + \cdots + & x_{k,n-1} & = & kn_k, \\
x_{k,k+1} & + & 2x_{k+1,k+1} & + \cdots + & x_{k+1,n-1} & = & (k+1)n_{k+1}, \\
\multicolumn{7}{c}{\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots} \\
x_{k,n-1} & + & x_{k+1,n-1} & + \cdots + & 2x_{n-1,n-1} & = & (n-1)n_{n-1},
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x_{k,n-1} &+ x_{k+1,n-1} &+ \cdots + & 2x_{n-1,n-1} &= & (n-1)n_{n-1},
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$$n_k + n_{k+1} + \cdots + n_{n-1} = n,$$

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- $$n_k + n_{k+1} + \cdots + n_{n-1} = n,$$

$$x_{i,j} \le n_i n_j, \quad k \le i < j \le n-1,$$

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$$x_{i,i} \le \binom{n_i}{2}, \quad k \le i \le n-1,$$

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$$\begin{aligned}
2x_{k,k} + x_{k,k+1} + \cdots + x_{k,n-1} &= k n_k, \\
x_{k,k+1} + 2x_{k+1,k+1} + \cdots + x_{k+1,n-1} &= (k+1) n_{k+1}, \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
x_{k,n-1} + x_{k+1,n-1} + \cdots + 2x_{n-1,n-1} &= (n-1) n_{n-1},
\end{aligned}$$

- $$n_k + n_{k+1} + \cdots + n_{n-1} = n,$$

- $$x_{i,j} \le n_i n_j, \quad k \le i < j \le n-1,$$

- $$x_{i,i} \le \binom{n_i}{2}, \quad k \le i \le n-1,$$

$x_{i,j},\ n_i$ are non-negative integers, for $k \le i \le j \le n-1$.

The main results

- **Theorem 1.** *If* $k \geq \lceil k_0 \rceil$, *where* $k_0 = q_0(n-1)$, $q_0 \approx 0.088$ *is the unique positive root of equation* $q\sqrt{q} + q + 3\sqrt{q} - 1 = 0$ *and if* $G \in G(k,n)$, *then*

$$GA(G) \geq \frac{kn}{2}.$$

If k *or* n *are even, this value is attained by regular graphs of degree* k.

Extremal graph for $k \geq \lceil k_0 \rceil$

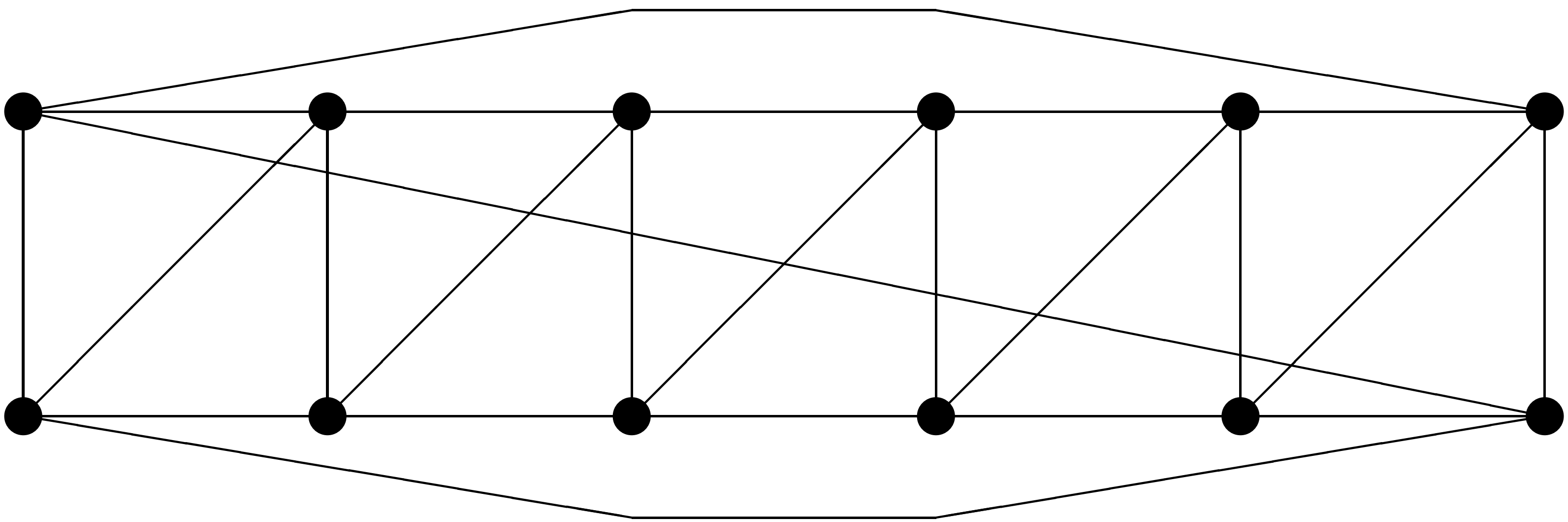

Fig. 1. Shape of extremal graph for $k = 4$.

Proof

- We will consider the problem of linear programming

$$\min\ GA(G) = \sum_{\substack{k\le i\le n-1\\ i\le j\le n-1}} \frac{2\sqrt{ij}}{i+j} x_{i,j}$$

subject to

$$\begin{array}{ccccccc}
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x_{k,n-1} & + & x_{k+1,n-1} & + \cdots + & 2x_{n-1,n-1} & = & (n-1)n_{n-1},
\end{array}$$

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x_{k,n-1} + x_{k+1,n-1} + \cdots + 2x_{n-1,n-1} &=& (n-1)n_{n-1},
\end{array}$$

$$n_k + n_{k+1} + \cdots + n_{n-1} = n,$$

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x_{k,n-1} + x_{k+1,n-1} + \cdots + 2x_{n-1,n-1} &=& (n-1)n_{n-1},
\end{array}$$

- $$n_k + n_{k+1} + \cdots + n_{n-1} = n,$$
-

$$x_{i,j} \ge 0, \quad k \le i \le j \le n-1, \qquad n_i \ge 0, \quad k \le i \le n-1.$$

Proof

- The basic variables are $n_i, \quad k \leq i \leq n-1$ and $x_{k,k}$.

$$n_i = \frac{x_{k,i} + \cdots + 2x_{i,i} + \cdots + x_{i,n-1}}{i}, \quad k+1 \leq i \leq n-1.$$

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$$n_i = \frac{x_{k,i} + \cdots + 2x_{i,i} + \cdots + x_{i,n-1}}{i}, \quad k+1 \le i \le n-1.$$

$$n_k = n - \sum_{i=k+1}^{n-1} \frac{1}{i} x_{k,i} - \sum_{k+1 \le i \le j \le n-1} \left(\frac{1}{i} + \frac{1}{j} \right) x_{i,j}.$$

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-

$$x_{k,k} = \frac{kn}{2} - \frac{1}{2} \sum_{i=k+1}^{n-1} \left(1 + \frac{k}{i} \right) x_{k,i} - \frac{1}{2} \sum_{k+1 \leq i \leq j \leq n-1} \left(\frac{k}{i} + \frac{k}{j} \right) x_{i,j}.$$

Proof

- Then

$$\begin{aligned} GA(G) &= \frac{kn}{2} + \sum_{i=k+1}^{n-1} \left(\frac{2\sqrt{ki}}{k+i} - \frac{k}{2}\left(\frac{1}{k} + \frac{1}{i}\right)\right) x_{k,i} \\ &+ \sum_{k+1 \le i \le j \le n-1} \left(\frac{2\sqrt{ij}}{i+j} - \frac{k}{2}\left(\frac{1}{i} + \frac{1}{j}\right)\right) x_{i,j}. \end{aligned}$$

Proof

- Since all $a_{i,j} \geq 0$ for $k \leq i \leq j \leq n-1$, we conclude that geometric-arithmetic index will attains its minimum value $\frac{kn}{2}$ if we put $x_{i,j} = 0$ for all $k \leq i \leq j \leq n-1$, except for $x_{k,k}$. Thus, we have proved

$$GA(G) \geq \frac{kn}{2}.$$

Geometric-arithmetic index attains minimum value $\frac{kn}{2}$ if k or n are even, on graphs for $x_{k,k} = \frac{kn}{2}$, $n_k = n$ and all other $x_{i,j} = 0$ and $n_i = 0$.

Case $n_k = n - 1$

- **Theorem 2.** *If* $n_k = n-1$ *and* $k \le \lfloor k_0 \rfloor$, *where* $k_0 = q_0(n-1)$, $q_0 \approx 0.0874$ *is the unique positive root of equation* $q^3 + 5q^2 + 11q - 1 = 0$, *then*

$$GA \ge \frac{(n-1)(k-1)}{2} + \frac{2(n-1)\sqrt{k(n-1)}}{k+n-1} = f_1.$$

If $(n-1)(k-1)$ *is even, the lower bound attains on graph* $G_{k,n-1}$ *which has* $n_{n-1} = 1$, $x_{k,n-1} = n-1$, $x_{k,k} = \frac{(n-1)(k-1)}{2}$ *and all others* $x_{ij} = 0$.

Extremal graph for $n_k = n - 1$

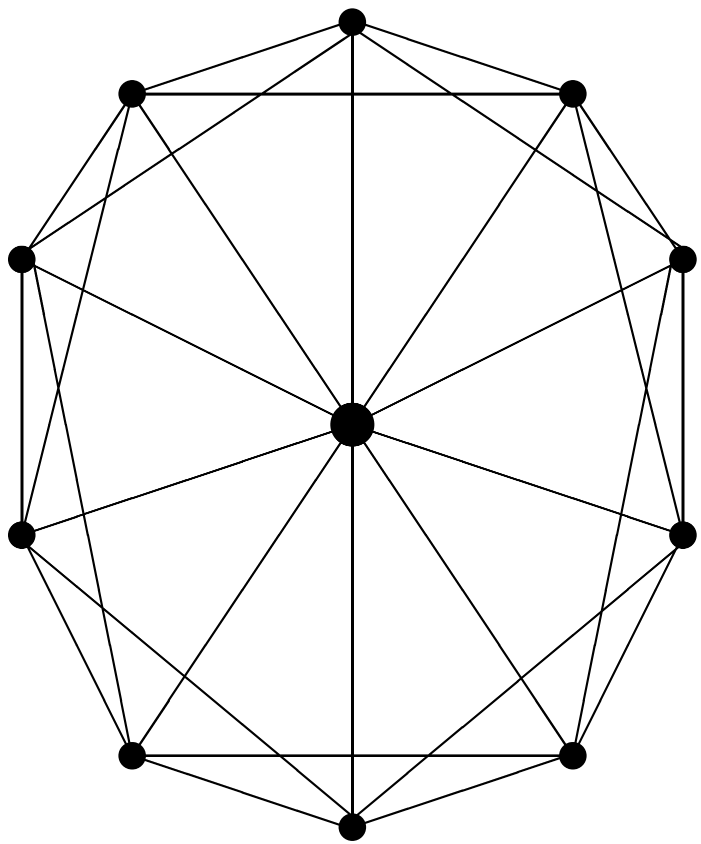


Fig. 2. Shape of extremal graph for $k = 5$.

Proof of Case $n_k = n - 1$

- In this case $n_{k+1} + \cdots + n_{n-1} = 1$, which implies that exists $k+1 \leq j \leq n-1$, such that $n_j = 1$. If $n_k = n-1$, then $x_{k,k} \geq \frac{n_k(n_k - n + k)}{2} = \frac{(n-1)(k-1)}{2}$. Put $x_{k,k} = \frac{(n-1)(k-1)}{2} + y_{k,k}$. We have

$$\begin{array}{rcrcl} 2x_{k,k} & + & x_{k,j} & = & kn_k, \\ x_{k,j} & + & 2x_{j,j} & = & jn_j. \end{array}$$

Proof of Case $n_k = n-1$

- In this case $n_{k+1} + \cdots + n_{n-1} = 1$, which implies that exists $k+1 \leq j \leq n-1$, such that $n_j = 1$. If $n_k = n-1$, then $x_{k,k} \geq \frac{n_k(n_k-n+k)}{2} = \frac{(n-1)(k-1)}{2}$. Put $x_{k,k} = \frac{(n-1)(k-1)}{2} + y_{k,k}$. We have

$$\begin{aligned} 2x_{k,k} &+ x_{k,j} &= kn_k, \\ x_{k,j} &+ 2x_{j,j} &= jn_j. \end{aligned}$$

- After substitution of $x_{k,k}$, and since $x_{j,j} = 0,\ n_j = 1$, we get

$$\begin{aligned} 2y_{k,k} &+ x_{k,j} &= (n-1), \\ x_{k,j} & &= j. \end{aligned}$$

We have $y_{k,k} = \frac{n-1-j}{2}$ and $x_{k,k} = \frac{(n-1)(k-1)}{2} + \frac{n-1-j}{2}$.

Proof of Case $n_k = n - 1$

- Geometric-arithmetic index is:

$$GA = \frac{(n-1)(k-1)}{2} + \frac{n-1-j}{2} + \frac{2j\sqrt{kj}}{k+j}$$

Proof of Case $n_k = n - 1$

- Geometric-arithmetic index is:

$$GA = \frac{(n-1)(k-1)}{2} + \frac{n-1-j}{2} + \frac{2j\sqrt{kj}}{k+j}$$

- Since $\frac{\partial^2 GA}{\partial j^2} \leq 0$, $\quad GA(j)$ is concave function for $j \geq k$ and attains its minimum value for $j = n-1$ or $j = k$,

$$GA(n-1) = \frac{(n-1)(k-1)}{2} + \frac{2(n-1)\sqrt{k(n-1)}}{k+n-1} = f_1,$$

$$GA(k) = \frac{nk}{2} = f_0.$$

Proof of Case $n_k = n - 1$

- $$f_1 - f_0 = \frac{-(n-1+k)^2 + 4(n-1)\sqrt{k(n-1)}}{2(k+n-1)}.$$

Proof of Case $n_k = n - 1$

- $$f_1 - f_0 = \frac{-(n-1+k)^2 + 4(n-1)\sqrt{k(n-1)}}{2(k+n-1)}.$$

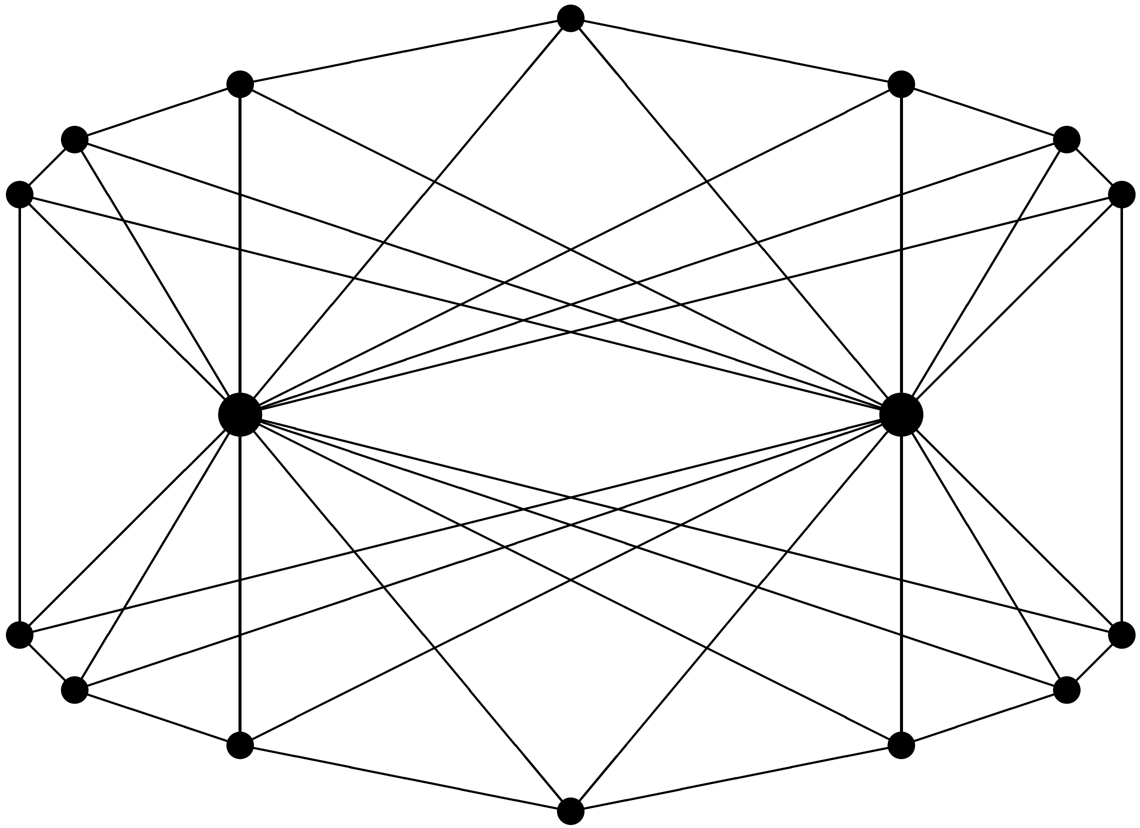
- $f_1 - f_0 \le 0$ if $k \le \lfloor k_0 \rfloor$, where $k_0 = q_0(n-1)$, $q_0 \approx 0.0874$ is the unique positive root of equation $q^3 + 5q^2 + 11q - 1 = 0$, that is of $q\sqrt{q} + q + 3\sqrt{q} - 1 = 0$.

Case $n_k = n-2$

- **Theorem 3.** *If* $n_k = n-2$ *and* $k \leq \lfloor k_1 \rfloor$, *where* k_1, *is the unique positive root of equation* $f_2 - f_1 = 0$, *then*

$$GA \geq \frac{(n-2)(k-2)}{2} + \frac{2(n-2)\sqrt{k(n-1)}}{k+n-2} 2(n-2) = f_2.$$

If $(n-2)(k-2)$ *is even, the lower bound attains on graph* $G_{k,n-2}$ *which has* $n_{n-2} = 2$, $x_{k,n-2} = 2(n-2)$, $x_{k,k} = \frac{(n-2)(k-2)}{2}$ *and all others* $x_{ij} = 0$.



▶

Fig. 3. Shape of extremal graph for $k = 4$

Sketch of the proof of Theorem 3

- We consider three cases: $a)$ $n_{n-1} = 2,$ $b)$ $n_{n-1} = 1$ and $c)$ $n_{n-1} = 0$.

Sketch of the proof of Theorem 3

- We consider three cases: $a)\ n_{n-1} = 2,\ b)\ n_{n-1} = 1$ and $c)\ n_{n-1} = 0$.

- **2a.** In this case we have $x_{k,k} = \frac{(n-2)(k-2)}{2},\ x_{k,n-1} = 2(n-2),\ x_{n-1,n-1} = 1$. We get

$$GA_2 = \frac{(n-2)(k-2)}{2} + \frac{2\sqrt{k(n-1)}}{k+n-1} 2(n-2) + 1.$$

Sketch of the proof of Theorem 3

- **2b.** In this case there is $k+1 \leq j \leq n-2$, such that $n_j = 1$. Then $x_{k,k} = \frac{(n-2)(k-2)}{2} + y_{k,k},\ x_{k,n-1} = n_k n_{n-1} = n-2,\ x_{j,j} = 0,\ x_{j,n-1} = n_j n_{n-1} = 1.$

Sketch of the proof of Theorem 3

- **2b.** In this case there is $k+1 \le j \le n-2$, such that $n_j = 1$. Then $x_{k,k} = \frac{(n-2)(k-2)}{2} + y_{k,k},\ x_{k,n-1} = n_k n_{n-1} = n-2,\ x_{j,j} = 0,\ x_{j,n-1} = n_j n_{n-1} = 1$.

- Similarly as in the case $n_k = n-1$, GA attains minimum value $GA_1(k)$ for $j = k$ or $GA_1(n-2)$ for $j = n-2$.

$$GA_1(k) = \frac{(n-1)(k-1)}{2} + \frac{2(n-1)\sqrt{k(n-1)}}{k+n-1} = f_1,$$

$$GA_1(n-2) = \frac{(n-2)(k-2)}{2} + \frac{1}{2} + \frac{2\sqrt{k(n-2)}}{k+n-2}(n-3)$$
$$+\frac{2\sqrt{k(n-1)}}{k+n-1}(n-2) + \frac{2\sqrt{(n-2)(n-1)}}{n-2+n-1}.$$

Sketch of the proof of Theorem 3

- **2c.** We solve the next problem of linear programming

$$\min \sum_{k\le i\le j\le n-2} \frac{2\sqrt{ij}}{i+j} x_{ij}$$

$$\begin{array}{ccccccc} 2y_{k,k} & + & x_{k,k+1} & +\cdots+ & x_{k,n-2} & = & 2(n-2), \\ x_{k,k+1} & + & 2x_{k+1,k+1} & +\cdots+ & x_{k+1,n-2} & = & (k+1)n_{k+1}, \\ \multicolumn{7}{c}{\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots} \\ x_{k,i} & + & x_{k+1,i} & +\cdots+ & x_{i,n-2} & = & in_i, \\ \multicolumn{7}{c}{\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots} \\ x_{k,n-2} & + & x_{k+1,n-2} & +\cdots+ & 2x_{n-2,n-2} & = & (n-2)n_{n-2}, \end{array}$$

$$n_{k+1} + n_{k+2} + \cdots + n_{n-2} = 2$$

Sketch of the proof of Theorem 3

- We get

$$GA \geq \frac{(n-2)(k-2)}{2} + \frac{2\sqrt{k(n-2)}}{k+n-2} 2(n-2) = f_2.$$

Sketch of the proof of Theorem 3

- We get

$$GA \geq \frac{(n-2)(k-2)}{2} + \frac{2\sqrt{k(n-2)}}{k+n-2} 2(n-2) = f_2.$$

- Since $f_2 \leq GA_2$, $f_2 \leq f_1$ and $f_2 \leq GA_1(n-2)$, we get that f_2 is minimum value of GA index in this case.

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