Minimizing the eccentric connectivity index with fixed number of pending vertices

G. Devillez[1] P. Hauweele[1] A. Hertz[2] H. Mélot[1]

[1]Université de Mons, Service d'Algorithmique

[2]Polytechnique Montréal - GERAD

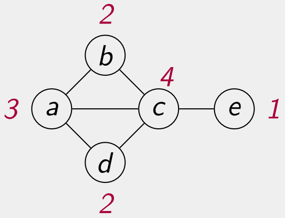
JGA 2019

Introduction

We consider simple undirected graphs. Let v be a vertex of a graph G, recall that:

- degree $d_G(v)$ = number of adjacent vertices of v;

Example

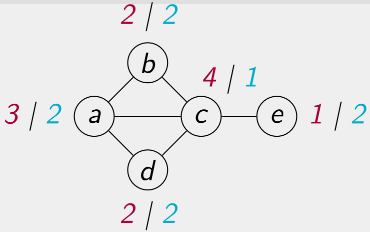


Introduction

We consider simple undirected graphs. Let v be a vertex of a graph G, recall that:

- degree $d_G(v)$ = number of adjacent vertices of v;
- eccentricity $\epsilon_G(v)$ = maximal distance between v and any other vertex.

Example



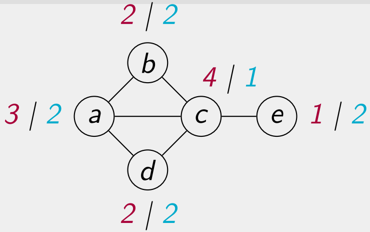
Introduction

We consider simple undirected graphs. Let v be a vertex of a graph G, recall that:

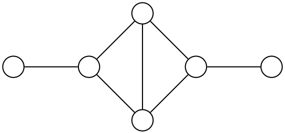
- degree $d_G(v)$ = number of adjacent vertices of v;
- eccentricity $\epsilon_G(v)$ = maximal distance between v and any other vertex.

We also define $w_G(v) = \epsilon_G(v) d_G(v)$.

Example



Introduction



For a graph $G = (V, E)$,

- its order $|V|$ is denoted by n;
- its number of pending vertices $P = |\{v \in V | d_G(v) = 1\}|$ is denoted by p.

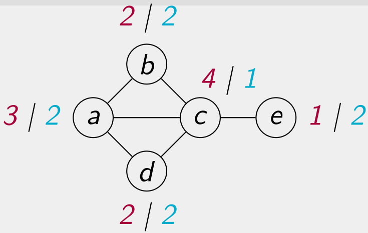
Eccentric Connectivity Index

Definition

The Eccentric Connectivity Index (ECI) of a graph G, denoted by $\xi^c(G)$, is

$$\xi^c(G) = \sum_{v \in V} d_G(v)\epsilon_G(v) = \sum_{v \in V} w_G(v).$$

Example



$$\xi^c(G) = 3 \times 4 + 2 + 6 = 20$$

Eccentric Connectivity Index

- Introduced by Sharma *et al.* in 1997 as a novel topological descriptor for molecules.
- Used in studies about anti-inflammatory properties, soil sorption of pesticides, anti-HIV activity of molecules, ...
- Not many extremal results about ξ^c.
- The first extremal results appears in 2010.

The problem

We want to solve the following problem :

Problem

Among all connected graphs with n vertices and p pending vertices, what are the graphs with minimum value of ξ^c?

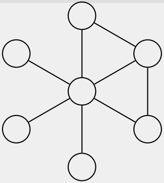
Note : in this talk, we only consider graphs with $n > 3$ and $p < n - 2$.

The graphs $H_{n,p}$

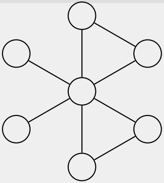
Definition

We define $H_{n,p}$ as the graph with n vertices and p pending vertices obtained from a star on n vertices by adding a maximal matching between $n-p-1$ pending vertices. If $n-p-1$ is odd, we add an edge between one of the remaining pending vertices and a vertex covered by the matching.

Example



$H_{7,3}$



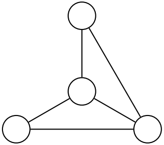
$H_{7,2}$

The graphs $H_{n,p}$

We can compute ξ^c $(H_{n,p})$ using the following formulae :

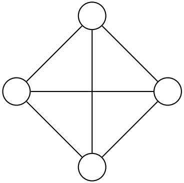
- If $n-p-1$ is even, $\xi^c(H_{n,p}) = 5n-2p-5$
- If $n-p-1$ is odd, $\xi^c(H_{n,p}) = 5n-2p-3$

Note : this doesn't work if $n=4$ and $p=0$ since $H_{4,0}$ has two dominant vertices. In this case, $\xi^c(H_{4,0}) > \xi^c(K_4)$.



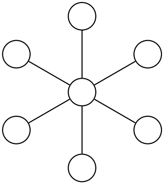
$\xi^c(H_{4,0}) = 14$

$>$



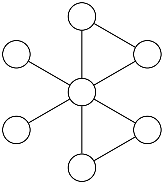
$\xi^c(K_4) = 12$

One dominant vertex



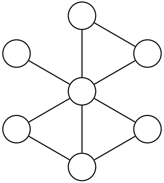
- At least a star on n vertices.

One dominant vertex



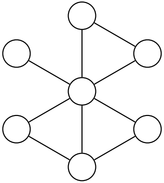
- At least a star on n vertices.
- We keep degrees as small as possible.

One dominant vertex



- At least a star on n vertices.
- We keep degrees as small as possible.
- We might need one additional edge.

One dominant vertex



- At least a star on n vertices.
- We keep degrees as small as possible.
- We might need one additional edge.
- This is $H_{n,p}$.

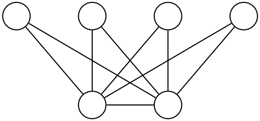
$x \geq 2$ dominant vertices

- With more than one dominant vertex, no pending vertex.
- Let G be such a graph :

$$\xi^c(G) \geq (n-1)x + (n-x)2x = -2x^2 + x(3n-1)$$

- Minimized when $x = 2$ or $x = n$.

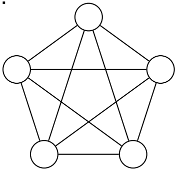
- $x = 2$:



$S_{n,2}$

$\xi^c(G) \geq 6n - 10$

- $x = n$:



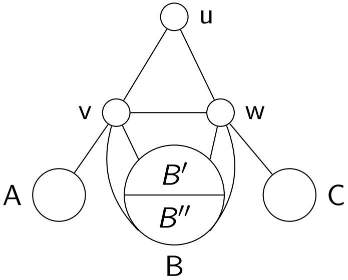
K_n

$\xi^c(G) \geq n^2 - n$

No dominant vertex

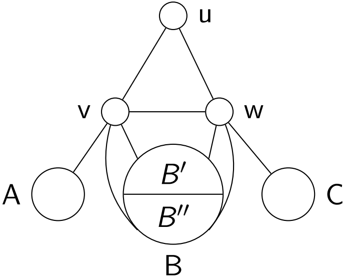
- Let $G = (V, E)$ be a graph with no dominant vertex, can it be as good as a graph with at least one dominant vertex ?
- We can show that $\exists u \in V$ such that $d_G(u) = \epsilon_G(u) = 2$
- Let v and w be the neighbors of u.
- We first suppose that v is adjacent to w.

- Let
  - $A = N(v) \backslash N(w) \backslash \{u, w\}$,
  - $C = N(w) \backslash N(v) \backslash \{u, v\}$,
  - $B = N(w) \cap N(v) \backslash \{u\}$,
  - $B' = \{x \in B | d_G(x) = 2\}$,
  - $B'' = B \backslash B'$.

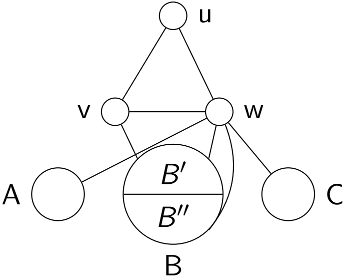


v and w are adjacent

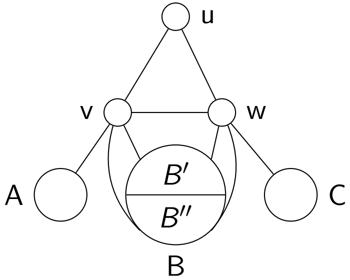
We obtain G' by applying the following transformation :



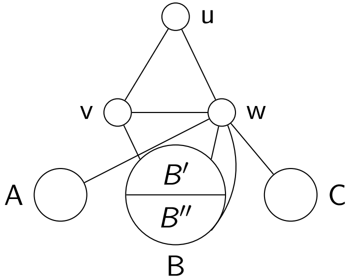
$\Rightarrow$



v and w are adjacent



$\Rightarrow$



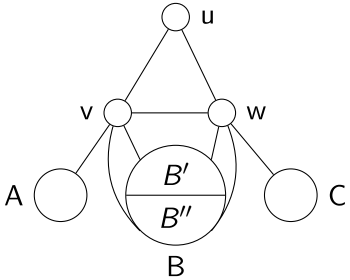
- We can show that

$$\sum_{z \in A \cup B \cup C \cup \{u\}} w_G(z) \geq \sum_{z \in A \cup B \cup C \cup \{u\}} w_{G'}(z)$$

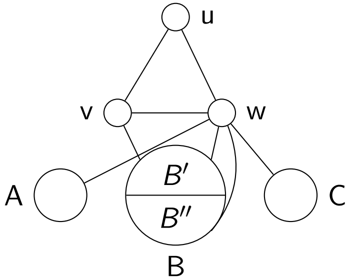
- Thus, to prove that G is not optimal, we have to show that

$$w_G(v) + w_G(w) - w_{G'}(v) - w_{G'}(w) = \alpha - \beta > 0$$

v and w are adjacent



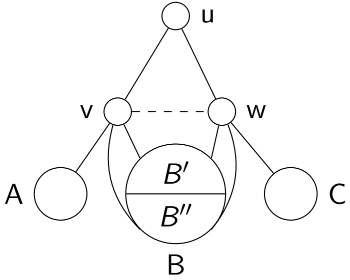
$\Rightarrow$



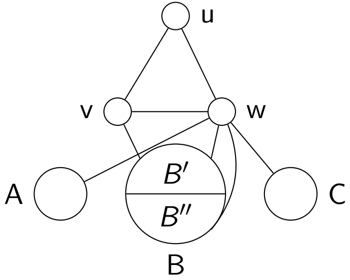
- $w_G(v) = 2(|A| + |B| + 2)$
- $w_G(w) = 2(|B| + |C| + 2)$
- $\alpha = 2\,|A| + 4\,|B| + 2\,|C| + 8$
- $w_{G'}(v) = 2(|B'| + 2)$
- $w_{G'}(w) = |A| + |B| + |C| + 2$
- $\beta = |A| + |B| + |C| + 2\,|B'| + 6$
- $\alpha - \beta = |A| + 3\,|B| - 2\,|B'| + |C| + 2 = |A| + |B'| + 3\,|B''| + |C| + 2 > 0$
- Thus G is not optimal.

v and w are not adjacent

If $A \cup B''$ and $C \cup B''$ are not empty, we obtain G' by applying the following transformation :

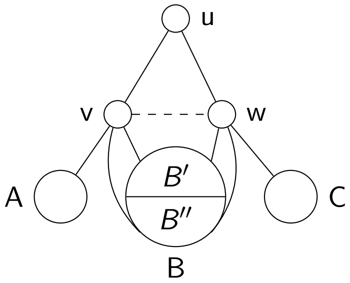


$\Rightarrow$

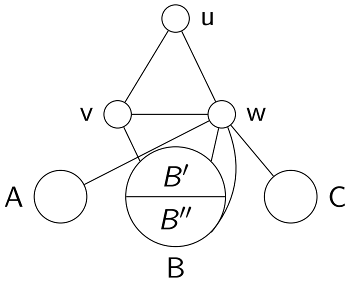


v and w are not adjacent

If $A \cup B''$ and $C \cup B''$ are not empty, we obtain G' by applying the following transformation :



$\Rightarrow$



- Just like before, we only need to show that $\alpha - \beta > 0$.
- But, $\alpha - \beta \geq |A| + |B'| + 3\,|B''| + |C| - 2 \geq 0$

When could G be optimal ?

$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

When could G be optimal ?

$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

- The set B'' must be empty.

When could G be optimal ?

$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

- The set B'' must be empty.
- B' must be empty too.

When could G be optimal ?

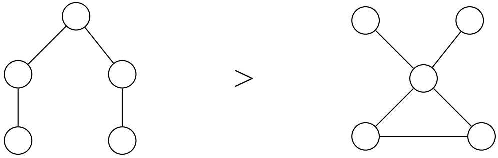
$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

- The set B'' must be empty.
- B' must be empty too.
- $|A| = |C| = 1$

When could G be optimal ?

$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

- The set B'' must be empty.
- B' must be empty too.
- $|A| = |C| = 1$
- Two possible non-improving situations :

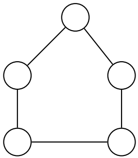


$\xi^c(P_5) = 24$ $>$ $\xi^c(H_{5,2}) = 16$

When could G be optimal ?

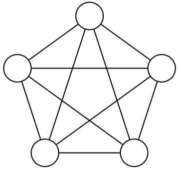
$$\alpha - \beta \geq |A| + \left|B'\right| + 3\left|B''\right| + |C| - 2$$

- The set B'' must be empty.
- B' must be empty too.
- $|A| = |C| = 1$
- Two possible non-improving situations :



$\xi^c(C_5) = 20$

$=$

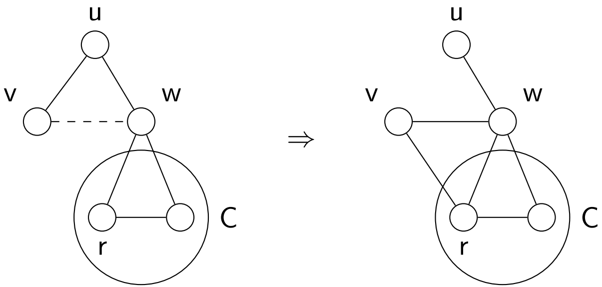


$\xi^c(K_5) = 20$

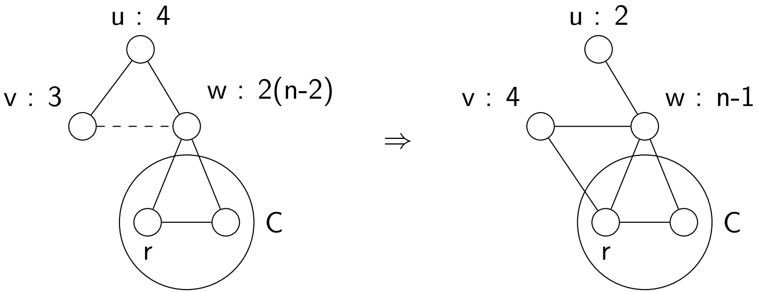
u and v are not adjacent

$A \cup B''$ (or $C \cup B''$) is empty

- If B' is empty, C is not empty since $n > 3$ and $\exists r \in C$ s.t. $d_G(r) \geq 2$ since $p \leq n - 3$.
- We can then apply the following transformation to obtain G' :



Changes in ξ^c

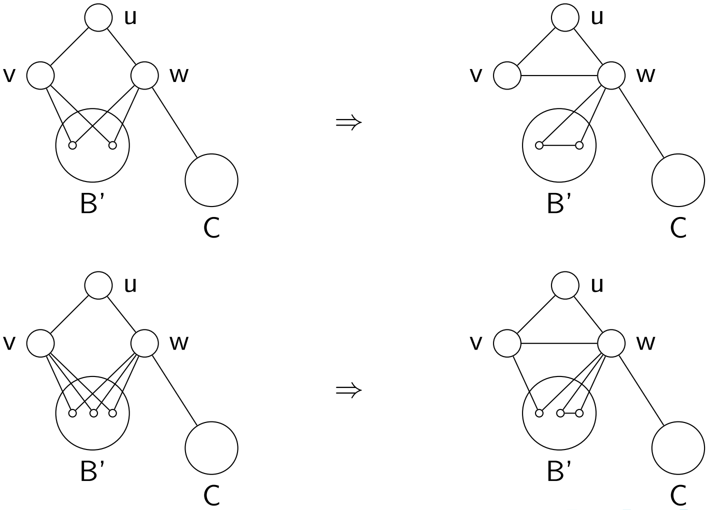


- $w_G(r) - w_{G'}(r) = 3d_G(r) - 2(d_G(r) + 1) = d_G(r) - 2$
- $\forall z \in C \backslash \{r\}, w_G(z) > w_{G'}(z)$
- There is at least one such vertex z such that $w_G(z) - w_{G'}(z) \geq 2$.
- Thus, $\xi^c(G) - \xi^c(G') \geq 2 - 1 + \underbrace{n-3}_{>0} + \underbrace{d_G(r) - 2}_{\geq 0} + 2 > 0$
- And G is not optimal.

u and v are not adjacent

$A \cup B''$ (or $C \cup B''$) is empty

- If B' is not empty, we transform G as follows :

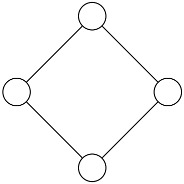


Conditions for optimality

- Again, we need to show that $\alpha - \beta > 0$ and again,

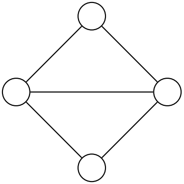
$$\alpha - \beta \geq 3\left|B'\right| + |C| - 4 \geq 0$$

- For G to be optimal, we need $|B'| = 1$ and $|C| \leq 1$.
- In these situations, the bound is actually too low and G' is still better :
- $|C| = 0$:



16

$>$



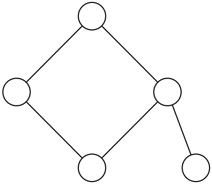
14

Conditions for optimality

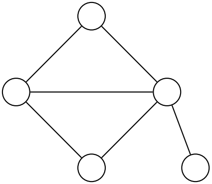
- Again, we need to show that $\alpha - \beta > 0$ and again,

$$\alpha - \beta \geq 3\left|B'\right| + |C| - 4 \geq 0$$

- For G to be optimal, we need $|B'| = 1$ and $|C| \leq 1$.
- In these situations, the bound is actually too low and G' is still better :
- $|C| = 1$:



$>$



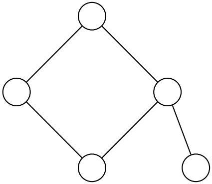
23 20

Conditions for optimality

- Again, we need to show that $\alpha - \beta > 0$ and again,

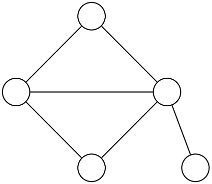
$$\alpha - \beta \geq 3\left|B'\right| + |C| - 4 \geq 0$$

- For G to be optimal, we need $|B'| = 1$ and $|C| \leq 1$.
- In these situations, the bound is actually too low and G' is still better :
- $|C| = 1$:



23

$>$

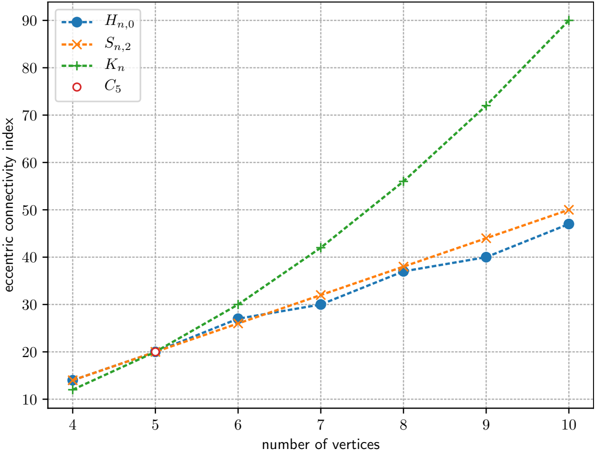


20

- In this case, G is again not optimal.

Comparison of results

- When $p > 0$, we saw that only $H_{n,p}$ is optimal.
- When $p = 0$, we can compare the different candidates we found numerically *via* the formulae :



Bibliography I

J. Zhang, Z. Liu, and B. Zhou.
On the maximal eccentric connectivity indices of graphs.
Appl. Math. J. Chinese Univ., 29:374 – 378, 2014.

Vikas Sharma, Reena Goswami, and AK Madan.
Eccentric connectivity index: a novel highly discriminating topological descriptor for structure- property and structure- activity studies.
Journal of chemical information and computer sciences, 37(2):273–282, 1997.

S Gupta, M Singh, and AK Madan.
Application of graph theory: Relationship of eccentric connectivity index and wiener's index with anti-inflammatory activity.
Journal of Mathematical Analysis and Applications, 266(2):259–268, 2002.

Bibliography II

P Gramatica, M Corradi, and V Consonni.
Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors.
Chemosphere, 41(5):763–777, 2000.

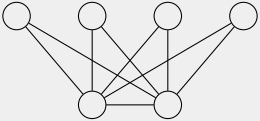
Vipin Kumar, Satish Sardana, and Anil Kumar Madan.
Predicting anti-hiv activity of 2, 3-diaryl-1, 3-thiazolidin-4-ones: computational approach using reformed eccentric connectivity index.
Journal of molecular modeling, 10(5-6):399–407, 2004.

The graphs $S_{n,2}$

Definition

We define $S_{n,2}$ as the graph with n vertices obtained from two adjacent vertices u and v by adding $n-2$ new vertices only adjacent to u and v.

Example

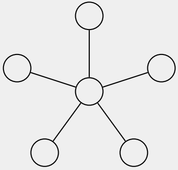


$S_{4,2}$

big values of p

- If $p = n - 1$, the graph can only be a star on n vertices.

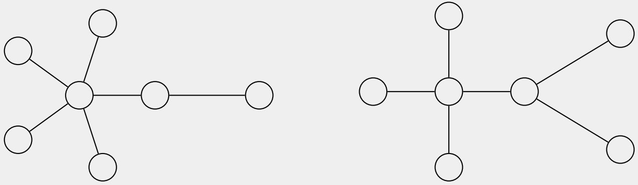
Example



big values of p

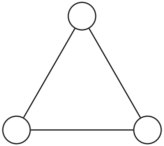
- If $p = n - 2$, the only possible graphs are obtained by adding $n - 2$ pending vertices randomly between the extremities of an edge with at least one pending vertex on each side.

Example



big values of p

In the rest of this talk, we suppose $p \leq n - 3$.
Note that if $n = 3$, we can only have $p = 0$ which is K_3.



We thus also suppose that $n \geq 4$.

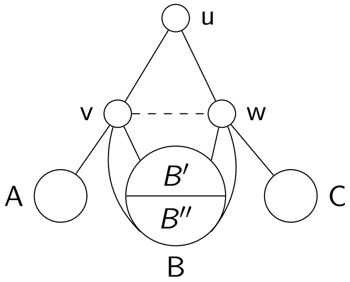
No dominant vertex

- Let G be an extremal graph with no dominant vertex.
- Let $Q \subseteq V$ be the set of vertices of degree 2 and eccentricity 2.
- If $Q = \emptyset$, G is not extremal:
  - Every non-pending vertex v has $d_G(v) \geq 2$ and $\epsilon_G(v) \geq 2$. And $d_G(v) \geq 3$ or $\epsilon_G(v) \geq 3$.
  - Every pending vertex v has $\epsilon_G(v) \geq 3$.
- Thus,

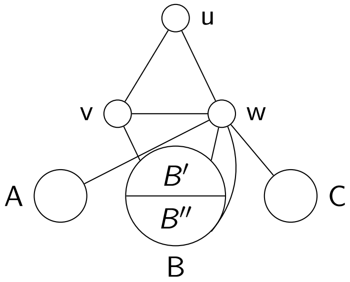
$$\xi^c(G) \geq 6(n-p) + 3p \geq 5n - 2p + 3 > \xi^c(H_{n,p})$$

- And G is not extremal.
- Also true when $n = 4$ and $p = 0$.

$A \cup B''$ and $C \cup B''$ are not empty



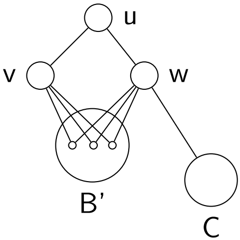
$\Rightarrow$



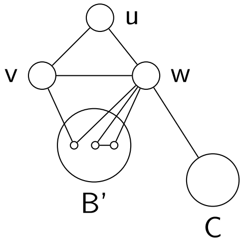
- $w_G(v) \geq 2(|A| + |B| + 1)$
- $w_G(w) \geq 2(|B| + |C| + 1)$
- $\alpha \geq 2\,|A| + 4\,|B| + 2\,|C| + 4$
- $w_{G'}(v) = 2(|B'| + 2)$
- $w_{G'}(w) = |A| + |B| + |C| + 2$
- $\beta = |A| + |B| + |C| + 2\,|B'| + 6$
- $\alpha - \beta \geq |A| + 3\,|B| - 2\,|B'| + |C| + 2 = |A| + |B'| + 3\,|B''| + |C| - 2$

Changes in ξ^c

- $\forall z \in B' \cup C \cup \{u\}, w_G(z) \leq w_{G'}(z)$



$\Rightarrow$



- $w_G(v) \geq 2(|B'| + 1)$
- $w_G(w) = 2(|B'| + |C| + 1)$
- $\alpha \geq 4\,|B'| + 2\,|C| + 4$

- $w_{G'}(v) \leq 6$
- $w_{G'}(w) = |B'| + |C| + 2$
- $\beta \leq |B'| + |C| + 8$

- $\alpha - \beta \geq 3\,|B'| + |C| - 4$

Comparison of results

We have the following results :

- If $p > 0$, $H_{n,p}$ is the extremal graph.
- If $n = 4$ and $p = 0$, the extremal graph is K_4.
- If $n = 5$ and $p = 0$, there are four extremal graphs : K_5, $H_{5,0}$, C_5 and $S_{5,2}$.
- If $n = 6$ and $p = 0$, the extremal graph is $S_{n,2}$.

Bounds for connected graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✗
m (size)	✓	✓
D (diameter)	✓	✓
p (number of pending vertices)	✓	✗
δ (minimum degree)	✗	✓
D (diameter) and m (size)	✓(with conditions on m and D)	
D' (degree distance)	✓	✗
M_1 (Zagreb index) and m	✗	✓
W (Wiener index)	✗	✓

Bounds for trees

Invariant(s)	Lower bound	Upper bound
—	✓	✓
D (diameter)	✓	✓
r (radius)	✗	✓
p (number of pending vertices)	✓	✓
Δ (maximum degree)	✓	✓
β (matching number)	✓	✓
α (stability number)	✓	✓
W (Wiener index)	✗	✓

Bounds for other graph classes

Unicyclic graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✓
g (girth)	✓	✓

Bicyclic graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✗

k-regular graphs

Invariant(s)	Lower bound	Upper bound
$k \geq 3$ fixed	✓	✓