Average Distance, Minimum Degree, and Irregularity Index

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Here...

In this talk we...

give an upper bound on the average distance of a connected graph of given order and minimum degree where irregularity index is prescribed.

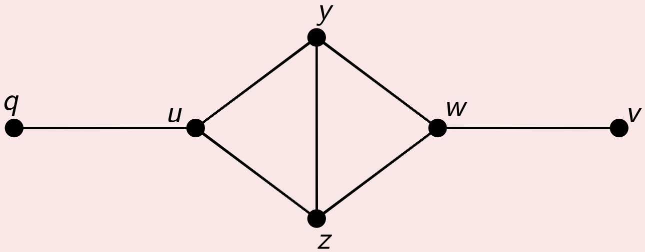
Our results are a strengthening of the classical theorems by:

- Kouider and Winkler (1997)
- Dankelmann and Entringer (2000).

Def:

Let $G = (V, E)$ be a connected graph.

- The degree, $\deg(v)$, of a vertex v in G is the number of vertices adjacent to v.
- The degree sequence, $DS(G)$, of G is a sequence of degrees of vertices of G.



Ex: (above) (i) $DS(G)$: 3,3,3,3,1,1. (ii) Minimum degree of G is $\delta(G) = \deg(v) = 1$.

Def:

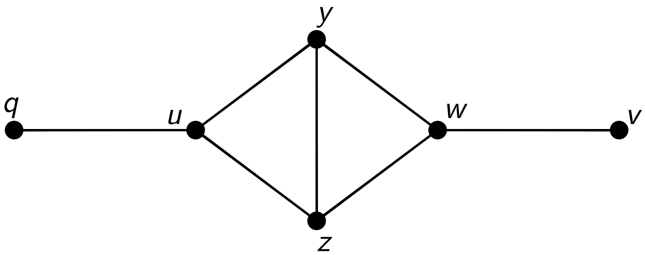
Let $G = (V, E)$ be a connected graph of order n.

- The distance $d(u, v)$ between vertices u and v in G is the length of a shortest u-v path in G.
- The average distance, $\mu(G)$, is

$$\mu(G) := \frac{\sum_{\{u,v\} \subseteq V} d(u, v)}{\binom{n}{2}}.$$

Variants (average distance):

transmission, average path length, mean distance, Wiener index.



Ex: (above)

- $d(v, z) = 2$,
- $\mu(G) = \frac{\sum_{\{u,v\} \subseteq V} d(u,v)}{\binom{n}{2}} = \frac{27}{\binom{6}{2}}$.

Folklore...

Theo:

Let G be a connected graph of order n. Then

$$\mu(G) \leq \frac{n+1}{3}.$$

Equality is attained iff G is a path.

Question:

Given that a graph has order n and minimum degree δ how how large can the average distance be?

A non-human mathematician, GRAFFITI, computer programme instructed by Fajtlowicz and Waller (1987):

Conjecture 62:

If G is a δ-regular graph of order n, then

$$\mu(G) \leq \frac{n}{\delta}.$$

Kouider and **Winkler** (1997): "*Conjecture 62...seems difficult to prove in the precise form stated.*"

Theo (Kouider and Winkler (1997)):

If G is a graph with n vertices and minimum degree δ, then

$$\mu(G) \leq \frac{n}{\delta+1} + 2.$$

By first developing a powerful method for finding a spanning tree with small average distance,

Theo (Dankelmann and Entringer (2000)):

Let G be a connected graph with n vertices and minimum degree δ. Then G has a spanning tree T with average distance at most

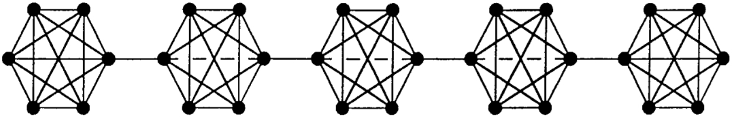
$$\mu(T) \leq \frac{n}{\delta+1} + 5.$$

Coro: (Dankelmann and Entringer (2000)):

Let G be a connected graph with n vertices and minimum degree δ. Then

$$\mu(G) \leq \frac{n}{\delta+1} + 5.$$

Extremal:



Recent discovery - drug design

geometrical shapes of compounds are important - "regular" keys sometimes do not unlock.

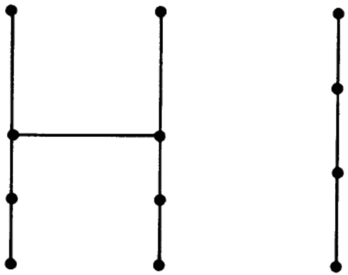
Chartrand, Erdös and Oellermann:

Question

How do you define irregularity in graphs?

Alavi, Chartrand, Chung, Erdös, Graham and Oellermann (1987):

(*opposite of regular graphs*):
A graph is highly irregular if it is connected and each of its vertices is adjacent only to vertices with distinct degrees.



More results...

- Alavi et al...showed: highly irregular graphs exist and are numerous.
- Majcher and Michael (1997): degree sequences of HI and HI graphs with extreme number of edges.

Concern:

Was the question "How do we define irregularity in graphs?" adequately answered?

M (2012): How far or near is a graph from being irregular or regular?

Def:

The irregularity index of a graph is the number of distinct terms in the graph's degree sequence.

A year later, **M (2013):**

Def:

A graph is maximally irregular if its irregularity index equals maximum degree.

Theo (M (2013)):

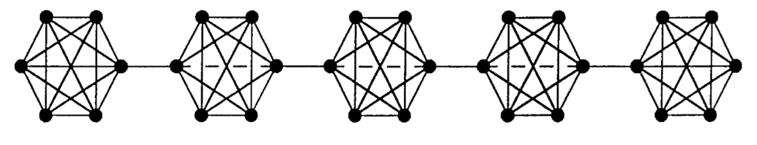
Every highly irregular graph is maximally irregular.

Some developments:

- Liu, Zhang and Meng (2014): studied size of maximally irregular and maximally irregular triangle–free graphs.
- Gutman (2016): criticized the use of irregularity index in chemistry.
- Horoldagva, Buyantogtokh, Dorjsembe and Gutman (2016): studied maximum size of maximally irregular graphs.
- M and Nyabadza (2021): discovered **correlation** between irregularity index & average distance and skin-cancer potency of compounds.
  - In particular, graphs with large average distance and certain irregularity index play an important role.

Rem:

The average distance extremal graph...



has very small irregularity index, 2.

Question: Given order, minimum degree and irregularity index, how large can average distance be, and what are the extremal graphs?

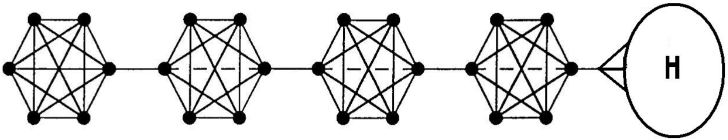
Theo (M (2022)):

Let G be a connected graph of order n, minimum degree δ and irregularity index t. Then

$$W(G) \leq \frac{(n-t)^3}{2(\delta+1)} + O(n^2).$$

Moreover, the bound is asymptotically best possible.

Extremal graph:



Graph H has minimum degree δ and irregularity index t.