

Nut graphs are not edge transitive

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Spectra of graphs

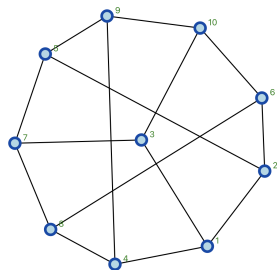
Let G be a finite simple graph of order n with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and let $E(G)$ denote the edge set of G .

The **adjacency matrix** of G is the matrix $A(G) = [a_{ij}]_{i,j=1}^n$, where

$$a_{ij} = a_{ji} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Example:

$$A(\text{GP}(5, 2)) = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$



Spectra of graphs

The **spectrum** of G , denoted $\sigma(G)$, is the multiset of eigenvalues of $A(G)$.

Examples:

$$\begin{aligned}\sigma(\text{GP}(5, 2)) &= \{3, 1^5, (-2)^4\} & \eta &= 0 \\ \sigma(K_{3,3}) &= \{3, 0^4, -3\} & \eta &= 4\end{aligned}$$

The exponents above give **multiplicity** of the eigenvalue, e.g. -2 is an eigenvalue of multiplicity 4 in $A(\text{GP}(5, 2))$. The multiplicity of the 0 eigenvalue is called **nullity** and denoted $\eta(G)$.

The eigenvalues are often ordered in non-increasing order

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n.$$

Graphs G and G' are called **cospectral** if $\sigma(G) = \sigma(G')$.

Singular and core graphs

A graph G is a **singular graph** if it has a zero eigenvalue.

The graph $K_{3,3}$ is singular, the graph $GP(5, 2)$ is non-singular.

A special class of singular graphs consists of the **core graphs**, graphs of which the kernel of the adjacency matrix contains a **full vector**. A full vector is a vector with no zero entry.

For example, the **kernel** (also called **null space**) of $A(K_{3,3})$ is

$$\ker A(K_{3,3}) = \text{span} \left\{ \mathbf{v}_1 = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \mathbf{v}_2 = \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \mathbf{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}, \mathbf{v}_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \right\}.$$

The local condition

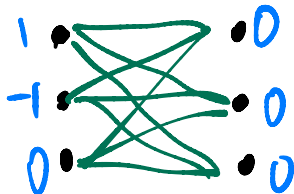
An eigenvector \mathbf{v} can be viewed as a weighting of vertices, i.e. a mapping $\mathbf{v}: V(G) \rightarrow \mathbb{R}$.

A vector $\mathbf{v} \in \ker A$ if and only if for each vertex $v \in V(G)$ the sum of entries over the open neighbourhood $N_G(v)$ equals 0:

$$\sum_{u \in N_G(v)} \mathbf{v}(u) = 0 \quad = \lambda \cdot \mathbf{v}(v)$$

The above equation is called the **local condition**.

Example ($K_{3,3}$):



Nut graphs

$$\eta \in \{0, 2, 4, 6, \dots\}$$

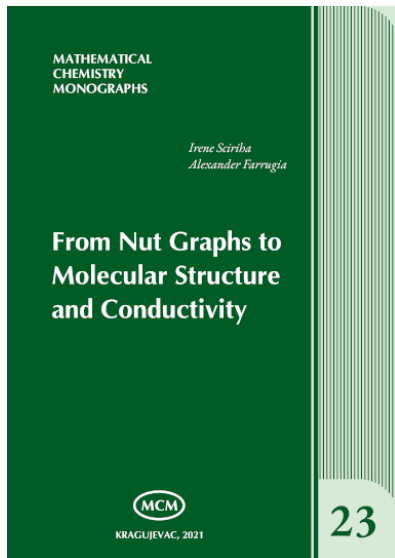
A simple graph G is a **nut graph** if G is a singular graph in which every non-zero vector in the kernel of $A(G)$ is full.

The term **nut graph** was coined in 1998 by Ivan Gutman and Irene Sciriha.

Here is an alternative (and, of course, equivalent) definition:

A simple graph G is a **nut graph** if G is a core graph with $\eta(G) = 1$.

Why nut graphs?

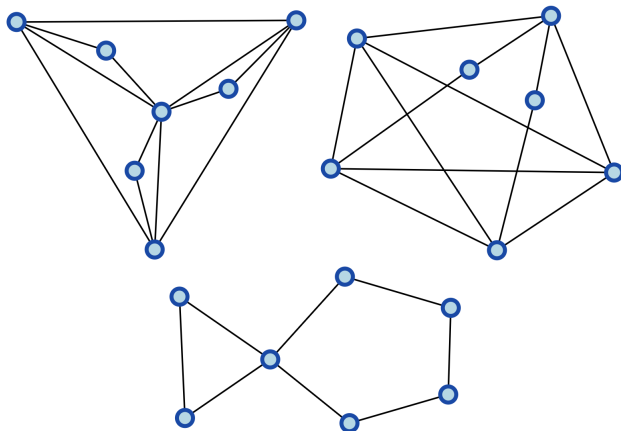


The smallest nut graphs (aka. Sciriha graphs)

Most authors require that a nut graph has $n \geq 2$ vertices.

K_1 could, in principle, be considered as the 'trivial' nut graph.

It is known that a nut graph must have at least 7 vertices.

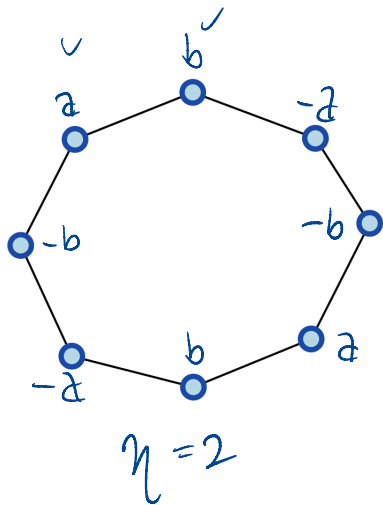
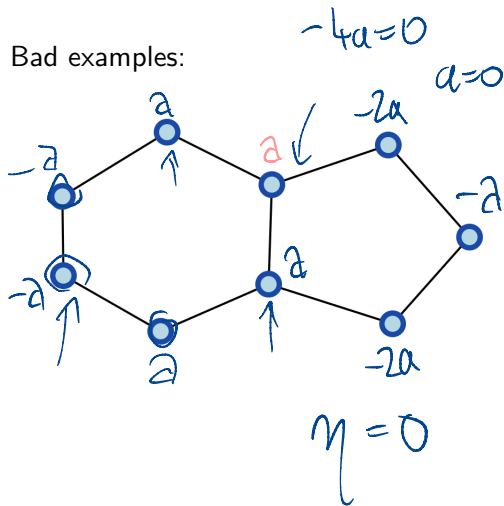


Pencil-and-paper method

Application of the local condition

$$\begin{aligned} a=0 & \quad b=1 \\ a=1 & \quad b=0 \end{aligned}$$

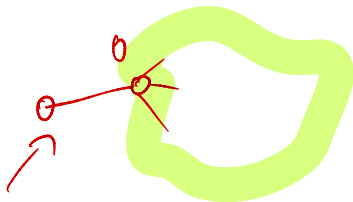
Bad examples:



Some properties of nut graphs

Some simple properties of nut graphs:

- 1 Every nut graph is **connected**.
- 2 Every nut graphs is **non-bipartite**.
- 3 Every nut graph is **leafless** (i.e. it have no vertices of degree one).



Number of nut graphs

Order	Nut graphs	Connected graphs	% of nuts
0 – 6	0	143	0.0000
7	3	853	0.0035
8	13	11117	0.0012
9	560	261080	0.0021
10	12551	11716571	0.0011
11	2060490	1006700565	0.0020
12	208147869	164059830476	0.0013
13	96477266994	50335907869219	0.0019

See <https://houseofgraphs.org/meta-directory/nut> for more.

Nut graph can be found in the following graph classes: [chemical graphs](#), [cubic graphs](#), [regular graphs](#), [planar graphs](#), [cubic polyhedra](#) (planar 3-connected), [fullerenes](#), ...

Constructions

Obtaining bigger nuts from smaller nuts

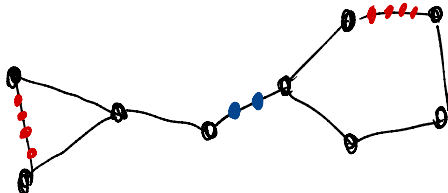
A few such constructions:

- 1 the bridge construction
- 2 the subdivision construction
- 3 the Fowler construction

$$\Delta \leq 3$$



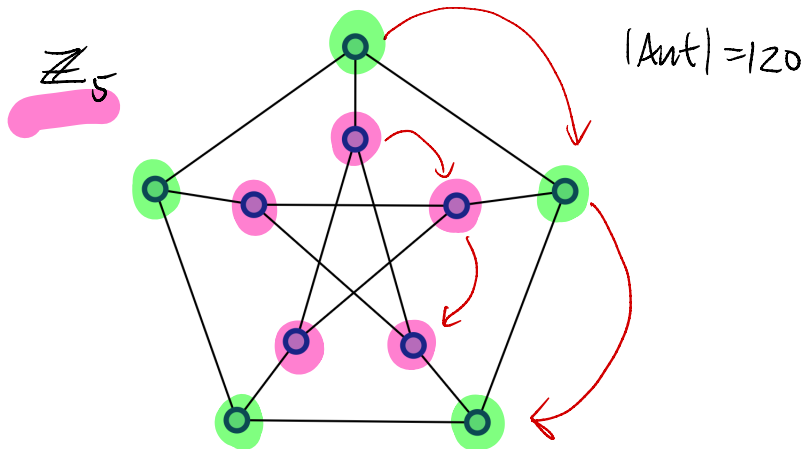
Example (smallest chemical nut graph):



Symmetry

Informally speaking

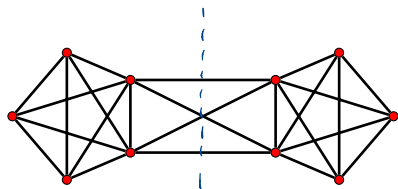
Can we rearrange the vertices somehow and still keep the same graph?



Symmetry

Full automorphism groups of nut graphs on 10 vertices

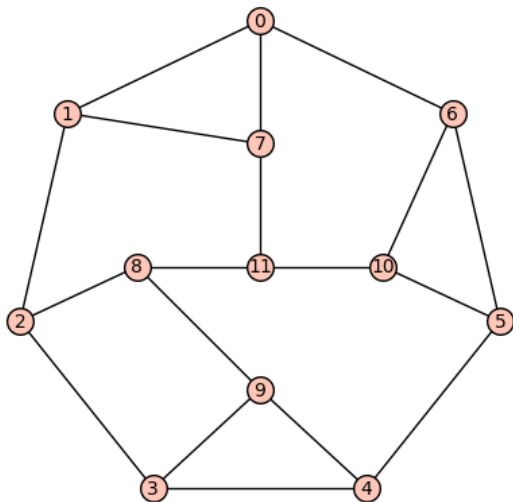
$ \text{Aut}(G) $	# graphs
1	8951
2	3101
4	394
6	9
8	58
10	1
12	19
16	5
20	1
24	3
32	3
36	2
48	2
72	1
288	1



$$3! \times 2 \times 2 \times 3! \times 2$$

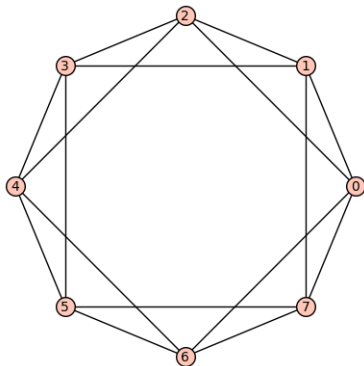
Frucht graph

One of the five smallest cubic asymmetric graphs



Vertex transitive nut graphs exist!

Vertex transitive (VT) nut graphs are graph with precisely one vertex orbit (v.r.t. the full automorphism group).



$\text{Circ}(8, \{1, 2\})$

What about edge-transitive nut graphs?

Edge transitive (ET) nut graphs are graph with precisely one edge orbit (v.r.t. the full automorphism group).

Census of ET graphs on orders $n \leq 47$ (by Conder and Verret).

- The census contains 1894 graphs in total. Of these, 335 graphs are non-singular and 2 graphs have nullity 1 (these graphs are K_1 and P_3).
- There are 1312 **core graphs** in the census (not counting K_1 as a core).
- Amongst these core graphs, there are 1098 bipartite graphs (945 non-regular graphs, 25 regular non-VT graphs and 128 VT graphs).
- The remaining 214 non-bipartite edge-transitive core graphs are necessarily VT, but none of these are nut graphs :~(

If they exist, what do they look like?

Lemma (Folklore)

Let G be an edge-transitive graph with no isolated vertices. If G is not vertex transitive, then $\text{Aut}(G)$ has exactly two orbits, and these two orbits are a bipartition of G .

The above lemma immediately implies:

Corollary

If H is an edge-transitive nut graph, then H is vertex transitive.

If they exist, what do they look like?

Theorem

Let G be a vertex-transitive nut graph on n vertices, of degree d . Then n and d satisfy the following conditions. Either

- $d \equiv 0 \pmod{4}$, and $n \equiv 0 \pmod{2}$ and $n \geq d + 4$; or
- $d \equiv 2 \pmod{4}$, and $n \equiv 0 \pmod{4}$ and $n \geq d + 6$.

It follows immediately that:

Corollary

If H is an edge-transitive nut graph, then H is vertex-transitive and of even degree and even order.

What else can we say about their structure?

Lemma

Let G be a vertex-transitive nut graph and let $\mathbf{x} = [x_1 \ \dots \ x_n]^T \in \ker A(G)$. Then the following statements hold:

- 1 $\mathbf{x} = \pm \mathbf{x}^\alpha$ for every $\alpha \in \text{Aut}(G)$;
- 2 $|x_i| = |x_j|$ for all i and j ;
- 3 we can take the entries to be $x_i \in \{+1, -1\}$.

The main result

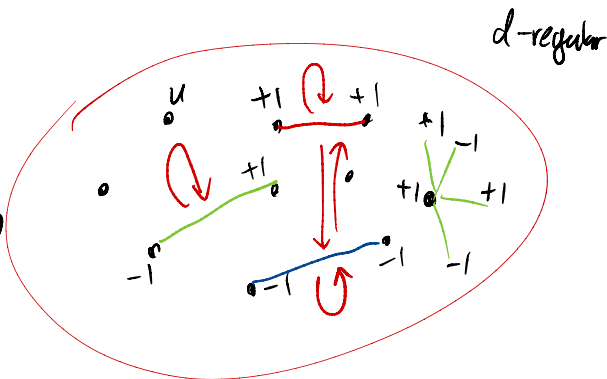
Theorem

Let G be a nut graph. Then G is not edge transitive.

Proof idea:

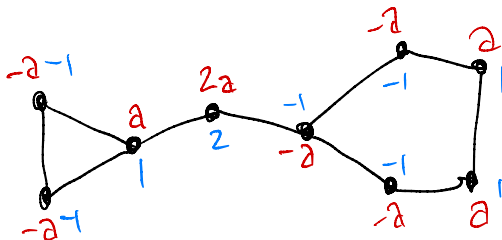
$$\sum_{u \in V(G)} \sum_{v \in N(u)} x(v) = 0$$

$$\parallel$$
$$\sum_{v \in V(G)} d \cdot x(v) = 0$$



Constructions & symmetry

Example: smallest chemical nut graph + bridge construction



Theorem

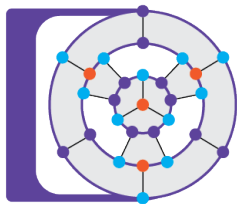
Let G be a nut graph. Then $o_e(G) \geq o_v(G) + 1$.

Long story short:

ET might want to phone home, but he is not a nut.



Thank you!



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Mathematical Chemistry

<https://dmc-journal.eu/>