AIM Workshop Spectra of Families of Matrices described by Graphs, Digraphs, and Sign Patterns Final Report: Mathematical Results (revised*)

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March 30, 2007

The workshop *Spectra of Families of Matrices described by Graphs, Digraphs, and Sign Patterns*, held at the American Institute of Mathematics Research Conference Center on Oct. 23-27, 2006, focused on three problems:

- Determination of the minimum rank, or equivalently maximum multiplicity of an eigenvalue, of real symmetric matrices described by a graph.
- The $2n$-conjecture for spectrally arbitrary sign patterns.
- The energy of graphs.

This report summarizes the mathematical results obtained at the workshop. For each of the three problems, there is a section that summarizes what was accomplished and provides background and notation used in the more detailed subsequent subsections, which are based on the written reports submitted by the working groups.

1 Minimum Rank of Symmetric Matrices described by a Graph

This report is based on the work of the following people: Francesco Barioli, Wayne Barrett, Avi Berman, Richard Brualdi, Steven Butler, Sebastian Cioaba, Dragoš Cvetković, Jane Day, Louis Deaett, Luz DeAlba, Shaun Fallat, Shmuel Friedland, Chris Godsil, Jason Grout, Willem Haemers, Leslie Hogben, In-Jae Kim, Steve Kirkland, Raphael Loewy, Judith McDonald, Rana Mikkelson, Sivaram Narayan, Olga Pryporova, Uri Rothblum, Irene Sciriha, Bryan Shader, Wasin So, Dragan Stevanović, Pauline van den Driessche, Hein van der Holst, Kevin Vander Meulen, Amy Wangsness, Amy Yielding.

Results

The workshop has already extended knowledge of the minimum rank in a variety of ways, and research continues in several directions developed at the workshop. The results already obtained

*This revision corrects minor errors in the report of November 17, 2006; it has not been updated to reflect developments since the workshop.

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are described in more detail in the following subsections, and can be loosely grouped into four types of results.

1. Examples and computation (§1.1, §1.2, §1.4). Minimum rank is regarded as a difficult graph parameter to compute (except for trees). Minimum rank of more than ten additional families of graphs was determined (beyond the few families for which minimum rank was already known). Software allowing easy computation of minimum rank for small graphs is being developed. A possible new upper bound, $\text{mr}(G) \leq |G| - \delta(G)$ where $\delta(G)$ is the minimum degree of G, is under investigation, and a better upper bound for the minimum rank for a bipartite graph has already been established. and a new upper bound for the minimum rank for a bipartite graph has already been established. The results of these efforts are being incorporated into an on-line catalog listing graphs, minimum rank and other graph parameters. This catalog will facilitate making and testing conjectures about minimum rank.

2. Effect of graph operations on minimum rank (§1.5, §1.6). The relationship between the minimum rank of a graph and its complement was investigated. All the examples in the catalog satisfy $\text{mr}(G) + \text{mr}(\overline{G}) \leq |G| + 2$. The relationship between minimum rank of a graph and its powers was studied and several results were obtained, including that for a tree T, $\text{mr}(T) - \text{mr}(T^2) \geq 1$, for a path the minimum rank of powers decreases steadily until it stabilizes at 2, and for a star, the minimum rank of powers oscillates.

3. Graphs having balanced inertia (§1.7). The ability to place the high multiplicity eigenvalue 0 in the middle of the spectrum played an important role in work on computing the effect of certain graph operations such as joins on minimum rank. It is not known whether all graphs are inertially balanced; all graphs in the catalog will be checked for balanced inertia. Properties of a minimal non-inertially balanced graph were determined. Related ideas involving raank strong vertices were investigated.

4. Minimum rank over fields other than $\mathbb{R}$ (§1.3). Before the workshop there was no known example where minimum rank over $\mathbb{R}$ is different than minimum rank over $\mathbb{Q}$ or $\mathbb{C}$. An example of a graph G has been constructed such that $\text{mr}^{\mathbb{Q}}(G) > \text{mr}^{\mathbb{R}}(G)$, and work continues on a related complex example. The topic of minimum rank over arbitrary fields received only limited attention and was delegated to a follow-up group that has begun work.

Background and Notation

As used here, the term *graph* means a simple undirected graph. Let G be a graph, denote the order of G by $|G|$, and let S_n denote the set of real symmetric $n \times n$ matrices. The *minimum rank* of G is

$$\text{mr}(G) = \min\{\text{rank}(A) : \ A \in S_n \text{ and for } i \neq j, \ a_{ij} \neq 0 \text{ if and only if } ij \text{ is an edge of } G\}.$$

Related questions involving symmetric matrices over an arbitrary field F were also invsestigated in some cases. Let $S_n(F)$ denote the set of symmetric $n \times n$ matrices ove F; the *minimum rank* of G is

$$\text{mr}(G) = \min\{\text{rank}(A) : \ A \in S_n(F) \text{ and for } i \neq j, \ a_{ij} \neq 0 \text{ if and only if } ij \text{ is an edge of } G\}.$$

The following two graph parameters are useful for a tree T: The *path cover number* $P(T)$ of T, is the minimum number of vertex disjoint paths occurring as induced subgraphs of T that cover all the vertices of T, and
$\Delta(T) = \max\{p - q : \text{there is a set of } q \text{ vertices whose deletion leaves } p \text{ paths}\}$.

Prior to the workshop, the following information was available for computation of minimum rank (for more information and original sources for these results, see the survey article on minimum rank being prepared by Shaun Fallat and Leslie Hogben based on workshop notes and slides).

1. Only connected graphs need be studied, as the minimum rank is the sum of the minimum ranks of the connected components.
2. For a tree T, $\mathrm{mr}(T) = |T| - \Delta(T) = |T| - P(T)$. There are good algorithms for computing $\Delta(T)$ and $P(T)$.
3. $\mathrm{mr}(P_n) = n - 2$, where P_n denotes the path on n vertices, and $\mathrm{mr}(G) = |G| - 1$ implies $G = P_{|G|}$.
4. $\mathrm{mr}(K_n) = 1$, where K_n denotes the complete graph on n vertices. For a connected graph G, $\mathrm{mr}(G) = 1$ implies $G = K_{|G|}$.
5. $\mathrm{mr}(C_n) = n - 2$, where C_n denotes the cycle on n vertices.
6. $\mathrm{mr}(K_{p,q}) = 2$, where $K_{p,q}$ denotes the complete bipartite graph on p, q vertices.
7. $\mathrm{mr}(G) \leq 2$ if and only if G does not contain one of a few specific graphs as an induced subgraph.
8. Graphs having minimum rank $|G| - 2$ have been characterized.
9. If G has a cut-vertex, the problem of computing the minimum rank of G can be reduced to computing minimum ranks of certain subgraphs.

The following notation will be used: The *complement* of a graph $G = (V, E)$ is the graph $\overline{G} = (V, \overline{E})$ whose set $\overline{E}$ of edges is the complement of E. The *Cartesian product* of two graphs G and H, denoted by $G \,\square\, H$, is the graph with vertex set $V(G) \times V(H)$ such that (u, v) is adjacent to (u', v') if and only if (1) $u = u'$ and $vv' \in E(H)$, or (2) $v = v'$ and $uu' \in E(G)$. The *strong product* of two graphs G and H, denoted by $G \boxtimes H$, is the graph with vertex set $V(G) \times V(H)$ such that (u, v) is adjacent to (u', v') if and only if (1) $uu' \in E(G)$ and $vv' \in E(H)$, or (2) $u = u'$ and $vv' \in E(H)$, or (3) $v = v'$ and $uu' \in E(G)$. Let $\pi(T)$ denote the number of pendent vertices in a tree T.

1.1 Minimum rank of special graphs

The following table will be part of an on-line catalog of minimum rank of selected graphs.

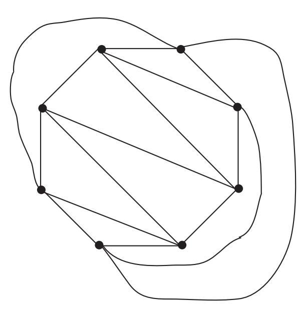

Figure 1: The planar 4-regular graph H_8

Table 1: Minimum rank of special graphs found at AIM workshop

	G	mr(G)	
1.	$C_n \,\square\, K_2 \quad (n \geq 4)$	$\lvert G\rvert - 4$	
2.	Möbius ladder $(n \geq 4)$	$\lvert G\rvert - 4$	
3.	$K_n \,\square\, K_2$ $(n \geq 2)$	n	
4.	$P_m \,\square\, P_n \quad (m \leq n)$	$(n-1)m$ if $\begin{cases} m \leq 4 \\ n = m \\ n = k(m+1)-1, \;\; k \in \mathbb{N} \end{cases}$	
5.	$P_m \boxtimes P_n$	$(n-1)(m-1)$	
6.	Q_n	2^{n-1}	
7.	$\overline{C_n} \quad (n \geq 5)$	$n-3$	
8.	$\overline{P_n}$	$n-3$	
9.	$L(K_n)$	$n-2$	
10.	$L(G)$	$n-2$	if G contains a Hamiltonian path, or G contains a $K_{k,n-k}$ with $1 < k < n-1$.
11.	$L(T)$, T a tree	$\lvert T\rvert - \pi(T)$.	
12.	H_8 (below)	4	

1.2 Computation of minimum rank

The property that $\mathrm{mr}^F(G) \leq k$ can be described by existential statements, as in the following know result.

Lemma 1.1. *Let G be a graph with vertices $1, \ldots, n$ and edge-set E, and let F be a field. Then the following are equivalent:*

(a) $\mathrm{mr}^F(G) \leq k$.

(b) The following statement is true over F:

$$\exists B = [b_{ij}] \in F^{n \times n}, x^1, \ldots, x^k, y^1, \ldots, y^k \in F^n$$
$$\bigwedge_{i,j=1}^{n} (b_{ij} = b_{ji}) \;\bigwedge (b_{ij} \neq 0 \;\forall i \neq j, \;\; ij \in E) \bigwedge (b_{ij} = 0 \;\forall i \neq j, \;\; ij \notin E)$$
$$\bigwedge (B = \sum_{i=1}^{k} x^i (y^i)^T).$$

(c) The following statement is true over F:

$$\exists B = [b_{ij}] \in F^{n \times n},$$
$$\bigwedge_{i,j=1}^{n} (b_{ij} = b_{ji}) \;\bigwedge (b_{ij} \neq 0 \;\forall i \neq j, \;\; ij \in E) \bigwedge (b_{ij} = 0 \;\forall i \neq j, \;\; ij \notin E)$$
$$\bigwedge (\det B[\alpha, \beta] = 0 \;\forall\; \alpha, \beta \subseteq \langle n \rangle \text{ with } |\alpha| = |\beta| = \mathrm{k} + 1).$$

(d) The following statement is true over F:

$$\exists B = [b_{ij}] \in F^{n\times n},$$
$$\bigwedge_{i,j=1}^{n} (b_{ij} = b_{ji}) \ \bigwedge (b_{ij} \neq 0 \ \forall i \neq j,\ ij \in E) \bigwedge (b_{ij} = 0 \ \forall i \neq j,\ ij \notin E)$$
$$\bigwedge (\det B[\alpha,\alpha] = 0 \ \forall\ \alpha \subseteq \langle n\rangle \text{ with } |\alpha| \geq \mathrm{k}+1).$$

Quantifier elimination allows one to verify the validity of statements of the form that appear in Lemma 1.1. Tarski observed that quantifier elimination can be done over the reals; in fact, Tarski produced an algorithm that does it. Quantifier elimination is even easier over the complex numbers. Algorithms have been improved over the years and software for verifying the validity of sentences (that are not too long) over the real or complex numbers is available.

Both *Mathematica* and *Maple* provide commands to determine whether existential statements are true. All these methods in Lemma 1.1 have been successfully implemented in *Mathematica* over the complex and real numbers for order 5 graphs, with the method (d) being the method of choice, and the only method likely to be viable for order larger than 5. We are consulting with an expert in high performance computing as to a better implementation. After improvements and testing, the minimum rank computation software will be made freely available on the web.

1.3 Minimum rank of over $\mathbb{Q}, \mathbb{R}, \mathbb{C}$

Since computations are easier to do over $\mathbb{C}$ than over $\mathbb{R}$, it is desirable to know whether $\mathrm{mr}^{\mathbb{C}}(G) = \mathrm{mr}^{R}(G)$ for all graphs. Clearly, $\mathrm{mr}^{\mathbb{R}}(G) \geq \mathrm{mr}^{\mathbb{C}}(G)$, but no example of a graph where the minimum rank was lower over $\mathbb{C}$ was known. This led to examination of the following question.

Question 1.2. *Does there exist a graph for which* $\mathrm{mr}^{\mathbb{R}}(G) > \mathrm{mr}^{\mathbb{C}}(G)$?

This lead also to a related question.

Question 1.3. *Does there exist a graph for which* $\mathrm{mr}^{\mathbb{Q}}(G) > \mathrm{mr}^{\mathbb{R}}(G)$?

The answers to these questions are also of interest in their own right. The following partial result was obtained.

Proposition 1.4. *Let G be a connected graph such that $|G| \leq 6$ and let F be an infinite field of characteristic not 2. Then $\mathrm{mr}^{F}(G) = \mathrm{mr}(G)$. In particular, $\mathrm{mr}^{\mathbb{Q}}(G) = \mathrm{mr}^{\mathbb{R}}(G) = \mathrm{mr}^{\mathbb{C}}(G)$.*

Through use of matroids, an example has been found that answers Question 1.3 in the affirmative, and work continues on a related example to answer Question 1.2.

In his early work on matroids, Saunders MacLane presented two interesting matrices. Let

$$S_1 = \begin{bmatrix} 1 & 0 & 1 & 0 & \omega & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1-\omega & 1 & -\omega \end{bmatrix},$$

where $\omega = \frac{-1+\sqrt{3}i}{2}$. and let

$$S_2 = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & \sqrt{2} & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & -1 & 2 & \sqrt{2} & \sqrt{2} & 1-\sqrt{2} \end{bmatrix}.$$

From a matrix A, a cycle matrix C_A is constructed that describes the dependence relations among the columns. A cycle matrix can be used to describe a zero-nonzero pattern for a family of matrices. The cycle matrices of the matrices S_1 and S_2 are used to give an example of a (not-symmetric) pattern such that the complex minimum rank of the family of matrices described by the pattern is less than the real minimum rank of the family of matrices described by the pattern, and an example of a (not-symmetric) pattern such that the real minimum rank of the family of matrices described by the pattern is less than the rational minimum rank of the family of matrices described by the pattern.

Lemma 1.5. *There is no real matrix T such that $C_T = C_{S_1}$.*

Theorem 1.6. $mr^{\mathbb{R}}(C_{S_1}) > mr^{\mathbb{C}}(C_{S_1})$.

Lemma 1.7. *There is no rational matrix T such that $C_T = C_{S_2}$.*

Theorem 1.8. $mr^{\mathbb{Q}}(C_{S_2}) > mr^{\mathbb{R}}(C_{S_2})$.

Note that these patterns are not symmetric, but are used to construct symmetric examples.

1.4 Upper and lower bounds for minimum rank and minimum degree

Prior to the workshop, the following bounds were known:

1. $\text{diam}(G) \le \text{mr}^F(G)$.
2. If p is the length (= # of edges) of the longest induced path of G, then $p \le \text{mr}^F(G)$.
3. If F is infinite, then $\text{mr}^F(G) \le \text{cc}(G)$ (where $\text{cc}(G)$ is the clique cover number of G).
4. If H is a minor of G and $\xi(H)$ is known, then it can be used to bound minimum rank: $mr^{\mathbb{R}}(G) \le |G| - \xi(H)$. This includes the following graphs H:
   (a) $\xi(K_p) = p - 1$
   (b) $\xi(K_{p,q}) = p + 1$ if $p <= q$ and $3 <= q$.

Item (2) gives a better bound than (1), which it implies, but (1) is easier to compute, and diameter is a well-known graph parameter. Item (4) is a consequence of minor monotonicity of the Colin de Verdière type parameter ξ but that applies only over the real numbers.

Other possible bounds for minimum rank derived from certain easy to compute parameters of the graph were considered, leading to an investigation of the connection between minimum degree of a vertex, $\delta(G)$, and minimum rank.

Conjecture 1.9. *For any graph G and infinite field F,*

$$\text{mr}^F(G) \le |G| - \delta(G).$$

Note that Conjecture 1.9 can be false for finite fields: $\text{mr}^{Z_2}(K_3 \,\square\, K_2) = 4 > 3 = |K_3 \,\square\, K_2| - \delta(K_3 \,\square\, K_2)$.

We have obtained the following results relating minimum rank and δ.

Proposition 1.10. *If $\delta(G) \le 3$ or $\delta(G) \ge |G| - 2$ then $\text{mr}^F(G) \le |G| - \delta(G)$.*

Corollary 1.11. *If $|G| \le 6$, then $\text{mr}(\mathcal{S}^F(G)) \le |G| - \delta(G)$.*

The graph H_8 in §1.1 is of interest. H_8 satisfies Conjecture 1.9 for the real numbers, but this is not a consequence of either Proposition 1.10 or the item 4, since $\delta(H_8) = 4$ but H_8 does not have a K_5 or $K_{3,3}$ minor.

Theorem 1.12. *For any bipartite graph G having bipartition $V(G) = U \cup W$,*

$$\mathrm{mr}^F(G) \leq 2(|U| - \delta_W(G) + 1) \text{ and } \mathrm{mr}^F(G) \leq 2(|W| - \delta_U(G) + 1).$$

where $\delta_W(G) = \min_{w \in W}\{\deg_G(w)\}$.

Corollary 1.13. *For any bipartite graph $G, \mathrm{mr}^F(G) \leq |G| - \delta(G)$.*

Theorem 1.14. *Let G be a connected graph with cut-vertex v and let $H_i, i = 1, \ldots, h$ be the connected components of $G - v$. If $\mathrm{mr}^F(H_i) \leq |H_i| - \delta(H_i)$ for all $i = 1, \ldots, h$, then* $\mathrm{mr}^F(G) \leq |G| - \delta(G)$.

Hence any possible counterexample to the δ-conjecture cannot be bipartite, and one of minimal order cannot have a cut-vertex.

Observation 1.15. *(Cf. Subection 1.5) If Conjecture 1.9 is true for regular graphs, a consequence would be that for any regular graph G,*

$$\mathrm{mr}^F(G) + \mathrm{mr}^F(\overline{G}) \leq |G| + 1.$$

Minimum rank of not-necessesarily symmetric matrices described by a graph was also investigated. A non -symmetric version of Conjecture 1.9 was established and used to prove the results on bipartite graphs.

1.5 Graph complements and minimum rank

The basic question considered concerning a graph and its complement is

Question 1.16. *How large can $\mathrm{mr}(G) + \mathrm{mr}(\overline{G})$ be? There are two possibilities:*

1. *Does there exist a constant $c \geq 2$ such that $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) \leq |G| + c$? If so find the smallest such c.*
2. *If not, find the best constant $d \leq 2$ such that $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) \leq d|G|$.*

Note that $c \geq 2$ by examination of a path (cf. §1.1) and $d \leq 2$ since $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) \leq 2|G| - 2$. All the special graphs in Section 1.1 for with the minimum rank of both G and $\overline{G}$ are known satisfy $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) \leq |G| + 2$. See also Observation 1.15.

Observation 1.17. *If G is a strongly regular graph then,*

$$\mathrm{mr}^F(G) + \mathrm{mr}^F(\overline{G}) \leq |G| + 1.$$

Graphs having $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) \leq 5$ are characterized ($|G| \geq 4$):

(1) $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) = 1$: Trivially implies that $G = K_n$ or $G_n = \overline{K_n}$.

(2) $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) = 2$: There can be no such G.

(3) $\mathrm{mr}(G) + \mathrm{mr}(\overline{G}) = 3$: Without loss of generality, $\mathrm{mr}(G) = 1$. Then $G = K_p \cup \overline{K_{n-p}}$ for some integer p with $2 \leq p \leq n - 1$, and $\overline{G} = \overline{K_p} \vee K_{n-p}$.

(4) $\text{mr}(G)+\text{mr}(\overline{G}) = 4$: Since both a graph and its complement cannot be disconnected, without loss of generality G is connected. Then

$$G = K_{s_1,s_2} \vee K_p \text{ or } (K_{s_1} \cup K_{s_2}) \vee K_p.$$

and

$$\overline{G} = (K_{s_1} \cup K_{s_2}) \cup \overline{K_p} \text{ or } K_{s_1,s_2} \vee K_p,$$

(5) $\text{mr}(G) + \text{mr}(\overline{G}) = 5$: Without loss of generality, $\text{mr}(G) = 2$. There are 4 possibilities for G:

(a) $G = (\overline{K_{s_1}} \cup (K_{p_1} \cup K_{q_1}) \vee K_t) \cup \overline{K_r})$,
(b) $G = (\overline{K_{s_1}} \vee \overline{K_{s_2}} \vee K_t) \vee \overline{K_r}$, (note that $\overline{K_{s_1}} \vee \overline{K_{s_2}} = K_{s_1,s_2}$)
(c) $G = ((K_{p_1} \cup K_{q_1}) \vee K_t) \cup \overline{K_r}$,
(d) $G = (K_{s_1} \vee K_t) \cup \overline{K_s}$.

1.6 Graph powers and minimum rank

Definition 1.18. *Let $G = (V, E)$ be a graph with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E. The j-th power of G is the graph $G^j = (V, F)$ where $\{u, v\} \in F$ if and only if there is a walk of length j from u to v.*

The basic question considered is:

Question 1.19. *What is the relationship between $\text{mr}(G)$ and $\text{mr}(G^j)$?*

Lemma 1.20. *Let G be a graph. Then $G^j \subseteq G^{j+2}$.*

We now focus our attention on trees.

Lemma 1.21. *Let P_n be the path on n vertices. Then $\text{mr}(P_n^j) \geq n - j$ for $1 \leq j \leq n - 2$.*

Theorem 1.22. *Let P_n be the path on n vertices with $n \geq 4$. Then $\text{mr}(P_n^j) = n - j$ when $1 \leq j \leq n-2$ and $\text{mr}(P_n^j) = 2$ for $j \geq n-2$. Moreover, this minimum is achieved at a nonnegative integer matrix.*

It thus follows from this theorem that the minimum ranks of powers of P_n ($n \geq 4$) start at $n-1$ and decrease by 1 each time until it reaches 2 at the $n-2$ power (when P_n^{n-2} is $K_{n/2} \cup K_{n/2}$ if n is even, and $K_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}$ when n is odd.) Notice that $P_3 = K_{1,2}$, the star on 3 vertices; the stars on n vertices, $K_{1,n-1}$, are described below. We have $\text{mr}(P_2^j)$ is 0 when j is even and 1 when j is odd.

It is well known that for a matrix M, $\text{rank}(M^j) \geq \text{rank}(M^{j+1})$. The following observation shows that $\text{mr}(G^j) \geq \text{mr}(G^{j+1})$ need not always hold.

Observation 1.23. *For the star on n vertices, $\text{mr}({K_{1,n-1}}^j)$ is 2 when j is odd and 1 when j is even.*

Open Problem 1.24. *Characterize the graphs G for which $\text{mr}(G^j) \geq \text{mr}(G^{j+1})$, for all $j \geq 1$.*

Theorem 1.25. *Let T be a tree on $n \geq 3$ vertices. Then $\text{mr}(T^2)$ is less than or equal to the number of non-pendent vertices.*

Note that the minimum rank of the line graph of a tree is also given by the number of non-pendent vertices (cf. §1.1).

Theorem 1.26. *For any tree T, $\pi(T) - P(T) \geq 1$.*

Corollary 1.27. *For any tree T, $\mathrm{mr}(T) - \mathrm{mr}(T^2) \geq 1$.*

The case of equality in the lower bound on $\pi(T) - P(T)$ has yet to characterized. It's clear that any path will provide an example for which equality holds in the lower bound.

Theorem 1.28. *Let T be a tree on at least 3 vertices; then $\pi(T) - P(T) \leq \frac{|T|}{3}$.*

Equality is attainable in the upper bound on $\pi(T) - P(T)$, for example by the tree on $3k$ vertices formed from P_k by adding $2k$ new vertices, and making each vertex of P_k adjacent to exactly 2 of the new vertices. A characterization of all trees yielding equality in the upper bound is still needed, however.

Conjecture 1.29. *If $T \neq K_{1,n-1}$, then $\mathrm{mr}(T^3) \leq \mathrm{mr}(T^2) - 1$.*

Question 1.30. *Is it the case that for each tree $T \neq K_{1,n-1}$, the sequence $\mathrm{mr}(T^j)$ decreases strictly until it hits its limit of 2?*

1.7 Inertially balanced graphs and rank spread

In order to determine the minimum rank for several classes of graphs (decomposable graphs, joins of graphs, ...) a central role is played by the relative position of the packet of zero eigenvalues in the spectrum of an optimal matrix. This fact leads to the notion of *balanced inertia*. More precisely, a matrix is said to be *inertially balanced* if $i_-(A) \leqslant i_+(A) \leqslant i_-(A) + 1$, where $i_+(A)$ is the number of positive eigenvalues of A, etc. Similarly, a graph is said to be inertially balanced if there exists an inertially balanced matrix A optimal for G, where a matrix $A \in \mathcal{S}(G)$ is *optimal* for G if $\mathrm{rank} A = \mathrm{mr}(G)$.

The following (classes of) graphs were known to be inertially balanced

1. trees;
2. n-cycles, $n \geqslant 3$;
3. decomposable graphs;
4. graphs with $\mathrm{mr}(G) \leqslant 2$;
5. graphs with $n \leqslant 4$ vertices.

Several new results were established:

Theorem 1.31. *If the minimum rank of G equals the clique cover number, then G is inertially balanced.*

Question 1.32. *Are all graphs inertially balanced?*

At present there are no examples of graphs that fail to be inertially balanced, and we suspect that the answer to Question 1.32 is yes.

Balanced inertia is strictly related to the notion of *rank-spread* of a graph G at a vertex v. Recall that the rank-spread is defined as $r_v(G) = \mathrm{mr}(G) - \mathrm{mr}(G - v)$, and it is well-known that $0 \leqslant r_v(G) \leqslant 2$. In particular a vertex v is said to be

- *rank null* if $r_v(G) = 0$;
- *rank weak* if $r_v(G) = 1$;

- *rank strong* if $r_v(G) = 2$.

Efforts to show all graphs are inertially balanced focused on determining necessary conditions for a minimal counter example. A graph G is *minimal non-inertially-balanced* if G is not inertially balanced, while all proper induced subgraphs of G are. A partial characterization of a minimal non-inertially balanced is provided by the following results.

Theorem 1.33. *A minimal non-inertially-balanced graph cannot have a rank-strong vertex.*

Theorem 1.34. *A minimal non-inertially-balanced graph cannot have pendent vertices.*

Theorem 1.35. *Let G have a vertex v such that the graph induced by the neighbors of v is a clique. If $r_v(G) \geqslant 1$ and $G - v$ is inertially balanced, then G is inertially balanced. In particular, a minimal non-inertially-balanced graph cannot have such a vertex.*

In view of Theorems 1.33 and 1.34, the existence of a sequence of rank-strong vertices provides a method for the construction of optimal inertially balanced matrices. Therefore, a natural question rises, namely, *do there exist graphs with only rank-strong vertices?* A similar question can be posed for graphs with only rank-null or only rank-weak vertices. A positive answer has been obtained for the last two questions. Indeed, in the complete graph K_n, $n \geqslant 3$, all vertices are rank-null, while an example of graph in which all the vertices are rank-weak is the Dart.

At present, the existence of graphs with all rank-strong vertices is still unknown.

2 Spectrally Arbitrary Patterns and the $2n$ Conjecture

This report is based on the work of the following people: Francesco Barioli, Louis Deaett, Luz DeAlba, David Farmer, Leslie Hogben, In-Jae Kim, Judith McDonald, Rana Mikkelson, Sivaram Narayan, Olga Pryporova, Bryan Shader, Pauline van den Driessche, Hein van der Holst, Kevin Vander Meulen, Amy Wangsness, and Amy Yielding.

Spectrally arbitrary sign patterns (or zero-nonzero patterns) allow every possible spectrum of a real matrix, or, equivalently, allow every monic real polynomial as the characteristic polynomial. Inertially arbitrary sign patterns (or zero-nonzero patterns) allow every possible inertia.

The $2n$-conjecture asserts that an $n \times n$ spectrally arbitrary pattern has at least $2n$ nonzero entries. It is known that a spectrally arbitrary $n \times n$ pattern must contain at least $2n - 1$ nonzero entries, and numerous examples of spectrally arbitrary $n \times n$ sign patterns with $2n$ nonzero entries are known. The $2n$-conjecture actually has four versions, the general and the irreducible versions for sign patterns and zero-nonzero (znz) patterns.

Conjecture 2.1. *(Irreducible $2n$ conjecture) Each irreducible $n \times n$ (sign or znz) pattern has at least $2n$ nonzero entries.*

Conjecture 2.2. *(General $2n$ conjecture) Each $n \times n$ (sign or znz) pattern has at least $2n$ nonzero entries.*

Obviously the general conjecture implies the irreducible conjecture, and for either conjecture, if it is true for znz patterns then it is true for sign patterns.

A number of participants suspect that the general conjecture is not true, and in fact one of the groups is working on a possible counterexample using a reducible pattern, whereas the consensus is that the irreducible $2n$ conjecture is true. Spectrally arbitrary patterns (SAPs) do not behave well under direct summation: The direct sum of two odd order SAPs is not an SAP, and there is an example of an SAP that is the direct sum of a non-SAP with an SAP.

It was suggested at the workshop that the general conjecture is incorrectly phrased. In an irreducible pattern, $n-1$ nonzero entries can be assumed to equal to 1, and thus at least $2n-1$ nonzero entries are needed to realize the n algebraically independent coefficients of the characteristic polynomial. Thus the irreducible conjecture could be rephrased to say that there is least one more nonzero entry than required to realize n algebraically independent coefficients. For a sign pattern with c irreducible components, $n-c$ of the entries can be assumed to be equal 1, and n other entries are needed to a realized the n algebraically independent coefficients. Thus the following revision of the general $2n$-conjecture is proposed:

Conjecture 2.3. *(Revised general $2n$ conjecture) Any $n \times n$ (sign or znz) pattern has at least $2n-c+1$ nonzero entries, where c is the number of irreducible components.*

There were three work groups for spectrally arbitrary patterns and their general topics were the following.

1. The irreducible $2n$ conjecture was investigated by exploring the proofs that an $n \times n$ irreducible, spectrally arbitrary sign (or zero-nonzero) pattern has at least $2n-1$ nonzero entries, and by studying generalizations and relaxations of the notion of a spectrally arbitrary pattern and the analogs of the $2n$-conjecture in these settings. An example of a zero-nonzero pattern that is a complex SAP but not a real SAP was found.

2. Reducibility issues: Construction of a possible counterexample to the general $2n$ conjecture by taking the direct sum of an SAP with $2n$ entries with an non-SAP with $2n-1$ entries was investigated, as was construction of possible examples of two non-SAPs whose direct sum in an SAP.

3. Full patterns that are SAPs or inertially arbitrary patterns (IAPs) were studied with the goals of finding a relatively simple necessary and sufficient condition for a full sign pattern to be spectrally (or inertially) arbitrary; and to find (if possible) a full sign pattern that is not spectrally (inertially) arbitrary, but that has a spectrally (inertially) arbitrary subpattern.

2.1 Irreducible patterns

Work on irreducible patterns focused on

> Developing a deeper understanding of the proofs that an $n \times n$ irreducible, spectrally arbitrary sign (or zero-nonzero) pattern has at least $2n-1$ nonzero entries with the hope that this would provide insight for a proof of the irreducible $2n$ conjecture.
>
> Exploring generalizations and relaxations of the notion of a spectrally arbitrary pattern and the analogs of the $2n$-conjecture in these settings.

The crux of each known proof that an $n \times n$ irreducible, spectrally arbitrary sign (or znz) pattern $\mathcal{A}$ has at least $2n-1$ nonzero entries is the simple fact that if a polynomial function $f : \mathbb{R}^k \to \mathbb{R}^n$ is surjective, then necessarily $k \geq n$. The particular polynomial function of interest for $\mathcal{A}$ is constructed by choosing a collection of $n-1$ nonzeros of $\mathcal{A}$ that correspond to a spanning tree in the graph of $\mathcal{A}$; setting $A(x_1, \ldots, x_m)$ to be the matrix with the chosen $n-1$ entries equal to 1 and the remaining $m-n+1$ nonzero entries being indeterminants $x_1, \ldots, x_{m-n+1}$; and defining then $f_{\mathcal{A}}(x_1, \ldots, x_{m-n+1}) = (p_1(x_1, \ldots, x_{m-n+1}), \ldots, p_n(x_1, x_2, \ldots, x_{m-n+1}))$ where $\det(xI - A) = x^n + p_1(x_1, \ldots, x_{m-n+1})x^{n-1} + \cdots + p_n(x_1, x_2, \ldots, x_{m-n+1})$. Note if $\mathcal{A}$ has exactly $m = 2n-1$ nonzero entries, then $f_{\mathcal{A}}$ is a polynomial map from $\mathbb{R}^n$ to $\mathbb{R}^n$, and then validity of the irreducible $2n$-conjecture is equivalent to the assertion that no such $f_{\mathcal{A}}$ is surjective. As there are surjective polynomial maps from $\mathbb{R}^n$ to $\mathbb{R}^n$, if the irreducible $2n$-conjecture is true, then it must be that the polynomial maps $f_{\mathcal{A}}$ have special properties. Some special properties of the $f_{\mathcal{A}}$ are listed in the following proposition.

Proposition 2.4. *Let $\mathcal{A}$ be an $n \times n$ irreducible, sign (or znz) pattern with $2n-1$ nonzero entries, and let $f_{\mathcal{A}}$ and $p_1, \ldots, p_n$ be defined as above. Then the following hold*

(a) $p_i(0, 0, \ldots, 0) = 0$ *for each* i.

(b) *deg*$(p_i) \leq i$ $(i = 1, 2, \ldots, n)$.

(c) The pre-image, $f_{\mathcal{A}}^{-1}((0, 0, 0, \ldots, 0))$, *of* $(0, 0, \ldots, 0)$ *has infinite cardinality.*

(d) Any collection of $k < n$ of $p_1, \ldots, p_n$ involves $k+1$ or more indeterminants.

(e) Each p_i is a sum or difference of distinct monomials.

Question 2.5. *What are necessary and sufficient conditions for a polynomial function f to equal $f_{\mathcal{A}}$ for some $\mathcal{A}$?*

Question 2.6.

Is there a surjective polynomial function $f : \mathbb{R}^n \to \mathbb{R}^n$ satisfying (a)-(e) of Proposition 2.4?

Question 2.7. *Is there anything special about f_A coming from* $\det(xI - A(x_1, \ldots, x_n))$ *rather than* $\chi(xI - A(x_1, \ldots, x_n))$ *where χ is an immanent (e.g. the permanent)?*

To gain additional insight into the $2n$-conjecture, the following related problem was posed and studied. Let $\mathcal{A}$ be a $n \times n$, sign (or zero-nonzero) pattern, and let $\beta = \{i_1, \ldots, i_k\}$ be a subset of $\{1, 2, \ldots, n\}$ of cardinality k. Then $\mathcal{A}$ is a *β-spectrally arbitrary pattern* provided for each k-tuple $(r_1, \ldots, r_k)$ of real numbers there is a realization A of $\mathcal{A}$ whose characteristic polynomial $x^n + \sum_{i=1}^{n} \alpha_i x^{n-i}$ satisfies $\alpha_{i_j} = r_j$ for $j = 1, 2, \ldots, k$. Known techniques can be extended to show that if $\mathcal{A}$ is an irreducible, $n \times n$ β-spectrally arbitrary pattern, then $\mathcal{A}$ has at least $n + |\beta| - 1$ nonzero entries.

Question 2.8. *Let k be a integer with $1 \leq k \leq n$. What is the minimum number of nonzero entries in an irreducible $n \times n$ sign (or znz) pattern which is β-arbitrary for some β with $|\beta| = k$?*

The analog of the $2n$-conjecture in this setting is:

Conjecture 2.9. *If $\mathcal{A}$ is an $n \times n$, β-spectrally arbitrary sign (or zero-nonzero) pattern, then $\mathcal{A}$ has at least $n + |\beta|$ nonzero entries.*

The notion of a spectrally arbitrary zero-nonzero pattern can be extended to an arbitrary field as follows. The $n \times n$, znz pattern $\mathcal{A}$ is a SAP over the field $\mathbb{F}$ provided that every monic polynomial of degree n in $\mathbb{F}[x]$ is the characteristic polynomial of some matrix with zero-nonzero pattern $\mathcal{A}$ and entries in $\mathbb{F}$. Exploration of analogs of spectrally arbitrary patterns and the $2n$-conjecture in various settings, yielded some basic results.

Theorem 2.10. *The $2n$-conjecture is true for zero-nonzero patterns over finite fields.*

The proof of Theorem 2.10 relies only on basic counting, and not on properties of polynomial functions, but does not seem to extend to infinite fields of nonzero characteristic.

Question 2.11. *Does every $n \times n$ zero-nonzero pattern over an infinite field of nonzero characteristic have at least $2n$ nonzero entries?*

Prior to the conference it was unknown whether or not the classes of spectrally arbitrary zero-nonzero patterns over the reals and over the complexes were different. The following example shows that they are different.

Example 2.12. *The zero-nonzero pattern*

$$A = \begin{bmatrix} * & * & 0 & 0 \\ * & 0 & * & 0 \\ 0 & 0 & * & * \\ * & 0 & 0 & * \end{bmatrix}.$$

is an SAP over $\mathbb{C}$, but is not SAP over $\mathbb{R}$.

2.2 Reducible patterns

Research in this subtopic was primarily concerned with two problems:

(a) Find, if possible, a reducible $n \times n$ SAP with fewer than $2n$ nonzero entries.

(b) Find, if possible, an SAP which is the direct sum of two non-SAPs. .

The recent discoveries of very sparse, reducible inertially arbitrary patterns and an SAP which is a direct sum of a non-SAP and an SAP, suggest that one might be able to use direct sums of non-SAPs to construct an $n \times n$ SAP with fewer than $2n$ nonzero entries.

The group worked on 6×6 zero-nonzero patterns with 11 nonzero entries, trying to determine whether any of them could be a component of a reducible SAP. Note if such a matrix could be direct-summed with an m by m matrix with $2m$ nonzero entries to obtain an SAP, then the desired example would be obtained.

An analysis of pattern

$$G_1 = \begin{bmatrix} \star & 0 & 0 & 0 & 0 & \star \\ 0 & \star & 0 & 0 & 0 & \star \\ 0 & \star & 0 & \star & 0 & 0 \\ 0 & 0 & 0 & 0 & \star & 0 \\ 0 & 0 & 0 & \star & 0 & \star \\ \star & 0 & \star & 0 & 0 & 0 \end{bmatrix}$$

shows the only characteristic polynomials not realized by G_1 have a very special form. Attempts to use this special form to show that G_1 could be a component of an $n \times n$ reducible SAP with $2n - 1$ nonzero entries (to date) have fallen tantalizing short, and continue.

In another direction, the known example of a non-SAP$\oplus$SAP that produces an SAP, was studied with the hope of finding some characteristics of such non-SAP patterns. Consider the sign-pattern

$$M_4 = \begin{bmatrix} + & + & - & 0 \\ - & - & + & 0 \\ 0 & 0 & 0 & - \\ + & + & 0 & 0 \end{bmatrix}$$

The characteristic polynomials that cannot be realized by M_4 are $p(x) = x^4 + b_3x^3 + b_2x^2 + b_0$, where either $b_0 = 0$ and $b_3^2 - 4b_2 < 0$, or $b_0 < 0$ and $b_3^2 - 4b_2 \leq 0$.

It was conjectured that all polynomials not realizable by M_4 have the same type of factorization over $\mathbb{R}$, namely fg_1g_2, where f is an irreducible quadratic and g_1 and g_2 are linear factors. In other words, the conjecture asserted that all polynomials not realizable by M_4 have exactly 2 real roots. However, the polynomial $x^4 + 1.95x^3 + x^2 - 0.05$ is not realizable by M_4 and has 4 real roots.

Surprisingly, for the zero-nonzero pattern associated with M_4, the conjecture is true, because the only polynomial not realizable by zero-nonzero pattern associated with M_4 is $x^4 + b_3x^3 + b_2x^2$ where $b_3^2 - 4b_2 < 0$, which is the product of x^2 and an irreducible quadratic.

A third direction of research focussed on finding a non-SAP zero-nonzero pattern P, such that the direct sum of it with M_4 is an SAP. One of the candidates for P was

$$C_4 = \begin{bmatrix} \star & \star & 0 & 0 \\ 0 & 0 & \star & \star \\ 0 & 0 & \star & \star \\ \star & \star & 0 & 0 \end{bmatrix}.$$

However, it was shown that $C_4 \oplus M_4$ is not SAP.

Based on comment made by the irreducible group in large group discussions (cf. Question 2.7), this group also worked on the permanental analog of SAPs. More precisely, an $n \times n$ sign pattern (or zero-nonzero pattern) $\mathcal{A}$ is *permanentally SAP*, provided every monic, real polynomial of degree n is $\text{per}(xI - A)$ for some $A \in \mathcal{A}$. The possibility of finding a permanentally arbitrary sign (or zero-non-zero) pattern that was not spectrally arbitrary was explored, using Mathematica. It was shown that there was no such 4×4 pattern, and work continues on the 5×5 patterns.

2.3 Full patterns

Full patterns, that is patterns with no zeros, that are SAPs or inertially arbitrary patterns (IAPs) were studied with the goals of finding a relatively simple necessary and sufficient condition for a full sign pattern to be spectrally (or inertially) arbitrary; and to find (if possible) a full sign pattern $\mathcal{A}$ such that $\mathcal{A}$ itself is not spectrally (inertially) arbitrary, but $\mathcal{A}$ has a spectrally (inertially) arbitrary subpattern.

Two necessary conditions for a sign pattern $\mathcal{A} = [\alpha_{ij}]$ to be inertially or spectrally arbitrary are:

(N1) There exist indices i, j such that $\alpha_{ii} = +$ and $\alpha_{jj} = -$; and

(N2) For some $i \neq j$, $\alpha_{ij}\alpha_{ji} = -$.

Since a full sign pattern has so much freedom in choosing values for its nonzero entries, it is natural to ask the following question:

Question 2.13. *Let $\mathcal{A}$ be a full $n \times n$ sign pattern. If $\mathcal{A}$ satisfies the necessary conditions* (N1) *and* (N2)*, then is $\mathcal{A}$ spectrally arbitrary? inertially arbitrary?*

When $n = 2$, the answers are yes. However, when $n = 3$, the full sign-pattern

$$\begin{bmatrix} - & + & + \\ - & + & - \\ - & - & + \end{bmatrix}.$$

satisifes (N1) and (N2) but is not potentially nilpotent, and the answers are no.

This leads to a modification of Question 2.13, which is yet to be resolved.

Question 2.14. *Let $\mathcal{A}$ be a full $n \times n$ sign pattern for $n \geq 4$. If $\mathcal{A}$ is a potentially nilpotent sign pattern with the two necessary conditions, then is $\mathcal{A}$ spectrally arbitrary?, inertially arbitrary?*

The primary technique used to demonstrate that a sign pattern is spectrally arbitrary is the Nilpotent-Jacobian (N-J for short) method that when applicable proves that every superpattern of the given pattern is spectrally arbitrary. It is not known in general whether or not every superpattern of a spectrally (resp. inertially) arbitrary sign pattern is spectrally (resp. inertially) arbitrary. However, it is known that a superpattern of an inertially arbitrary zero-nonzero pattern need not be inertially arbitrary.

Question 2.15. *Is there a spectrally (inertially) arbitrary sign pattern having a (full) superpattern that is not spectrally (inertially) arbitrary?*

It is known that the reducible pattern $\mathcal{T}_2 \oplus \mathcal{T}_2$ is spectrally arbitrary, where

$$\mathcal{T}_2 = \begin{bmatrix} + & + \\ - & - \end{bmatrix}.$$

However, the N-J method cannot be used to show that $\mathcal{T}_2 \oplus \mathcal{T}_2$ is spectrally arbitrary, since, at every nilpotent realization of a reducible sign pattern, the last row of the Jacobian corresponding to the constant term is always zero. Thus, it is not known whether or not every superpattern of $\mathcal{T}_2 \oplus \mathcal{T}_2$ is spectrally arbitrary. However, by using similarity transformations on matrices in $\mathcal{T}_2 \oplus \mathcal{T}_2$ one can show that

$$\mathcal{B} = \begin{bmatrix} + & + & - & - \\ - & - & + & + \\ + & + & + & + \\ - & - & - & - \end{bmatrix}$$

is spectrally arbitrary.

In the same way, Givens rotations appear useful in finding spectrally (inertially) arbitrary superpatterns of a spectrally arbitrary pattern. Using Givens rotations, certain superpatterns of $\mathcal{T}_2 \oplus \mathcal{T}_2$ were shown to be inertially arbitrary.

If all of the (full) superpatterns of $\mathcal{T}_2 \oplus \mathcal{T}_2$ turn out to be spectrally arbitrary, then the next pattern to investigate is $\mathcal{M}_4 \oplus \mathcal{T}_2$ in order to find a (full) superpattern that is not spectrally arbitrary, where

$$\mathcal{M}_4 = \begin{bmatrix} + & + & - & 0 \\ - & - & + & 0 \\ 0 & 0 & 0 & - \\ + & + & 0 & 0 \end{bmatrix}.$$

It is known that $\mathcal{M}_4$ is not spectrally arbitrary, but $\mathcal{M}_4 \oplus \mathcal{T}_2$ is spectrally arbitrary.

3 Energy of Graphs

This report is based on the work of the following people: Wayne Barrett, Avi Berman, Richard Brualdi, Steven Butler, Sebastian Cioaba, Dragoš Cvetković, Jane Day, Shaun Fallat, Shmuel Friedland, Chris Godsil, Jason Grout, Willem Haemers, Steve Kirkland, Raphael Loewy, Uri Rothblum, Irene Sciriha, Wasin So, Dragan Stevanović.

The energy of a graph (the sum of the absolute values of the eigenvalues of the adjacency matrix) has applications to chemistry. Certain quantities of importance to chemists, such as the heat of formation of a hydrocarbon, are related to pi-electron energy that can be calculated as the energy of an appropriate "molecular" graph. Recently the Laplacian energy of a graphs, the analogue of energy for the Laplacian matrix of G, has also been studied. The workshop investigated both the energy of a graph and the Laplacian energy. Both kinds of energy, depending as they do on all the eigenvalues of a matrix, are very difficult to work with.

As used here, the term *graph* means a simple undirected graph. Let $V(G)$ and $E(G)$ denote the vertex set and the edge set of a graph G.

1. **Energy**: This group focussed on the effect on energy of adding, removing, or subdividing an edge of a graph. A general result was proved which implied that removing an edge can change the energy by at most 2 and subdividing an edge can change it by at most 4. Also considered was the energy per vertex and its maximum $f(k)$ over all regular graphs of degree k with n vertices. If k is a prime power, then tight upper and lower bounds were obtained for $f(k+1)$ (using combinatorial configurations). Many new and interesting questions and conjectures arose, such as: (1) Are there any graphs for which the energy goes up by 2 when some edge is removed?, and (2) Is K_2 the only connected graph with an edge whose removal decreases the energy by 2?

2. **Laplacian Energy**: This is a recent concept defined to be the sum of the absolute values of the difference between the eigenvalues of the Laplacian matrix and the average degree of a vertex (equivalently, the average value of the eigenvalues). The group investigating Laplacian energy focussed on a conjecture that the vector of n eigenalues is majorized by the conjugate (in the sense of number theory) of the degree sequence, with equality for a class of extremal graphs known as threshold graphs, and its implications for Laplacian energy. There was a conjecture that maximum Laplacian energy was obtained by a special class of threshold graphs called pineapples. A disconnected counterexample was discovered but the conjecture remains open for connected graphs. The (strict) upper bound of $2m$ (m is the number of edges) was obtained for Laplacian energy. Many related questions were posed and discussed concerning this hard topic.

3.1 Energy

The energy of a graph G on n vertices with eigenvalues $\lambda_1, \dots, \lambda_n$ is

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$$

We analyzed the behavior of the energy when adding, removing or subdividing an edge. By subdividing an edge we mean replacing it with a path of length 2.

Theorem 3.1. *If G and H are graphs such that $V(G) = V(H)$ and $E(G) \cap E(H) = \emptyset$, then*

$$|\mathcal{E}(G) - \mathcal{E}(H)| \leq \mathcal{E}(G \cup H) \leq \mathcal{E}(G) + \mathcal{E}(H)$$

The graph $G \cup H$ has $V(G)$ as vertex set and $E(G) \cup E(H)$ as edge set.

Corollary 3.2. *If G is a graph and $e \in E(G)$, then*

$$|\mathcal{E}(G) - \mathcal{E}(G \setminus e)| \leq 2$$

Corollary 3.3. *If H is the graph obtained by subdividing an edge of a graph G, then*

$$|\mathcal{E}(G) - \mathcal{E}(H)| \leq 4$$

Lemma 3.4. *If $G \in \{K_n, P_n, C_n\}$, then subdividing an edge of G increases the energy.*

We are interested in determining

$$f(k) = \max \frac{\mathcal{E}(G)}{|V(G)|} \tag{1}$$

where the maximum is taken over all k-regular graphs on n vertices.
Without loss of generality, we can restrict ourselves to bipartite k-regular graphs.

Theorem 3.5. *If q is a prime power, then*

$$\sqrt{q} + \frac{1}{q + \sqrt{q} + 1} \leq f(q+1) < \sqrt{q} + \frac{1}{\sqrt{q+1} - \sqrt{q}}$$

The energy per vertex for the 3-regular graph obtained as a bipartite double cover of the incidence graph of the projective plane of order 2 (also known as the Heawood graph) is $\frac{6+3\sqrt{2}}{7} = 1.64705$. We have checked by computer that $\frac{6+3\sqrt{2}}{7}$ is larger than the energy per vertex of any other 3-regular graph on less than 22 vertices.

Open Problems

Conjecture 3.6. *If e is an edge of a connected graph G such that $\mathcal{E}(G) = \mathcal{E}(G \setminus e) + 2$, then $G = K_2$.*

Question 3.7. *Are there any graphs G such that*

$$\mathcal{E}(G \setminus e) = \mathcal{E}(G) + 2 \tag{2}$$

for some edge e of G ?

Question 3.8. *For what connected graphs G, is there an $e \in E(G)$ such that $\mathcal{E}(G \setminus e) = \mathcal{E}(G)$?*

Definition 3.9. *Let the diamond be the graph K_4 minus an edge. The central edge of a diamond is the edge between the two vertices of degree 3. If i is a vertex of a graph G, $\overline{N}(i)$ (the closed neighborhood of i) denotes the set of vertices adjacent to i in G and includes i.*

$$\overline{N}(i) = \{i\} \cup \bigcup_{ij \in E(G)} \{j\}.$$

If V is a set of vertices in G, then $G[V]$ is the induced subgraph of G induced by the vertices in V.

Conjecture 3.10. *Let G be a graph, ij be an edge in G, and H be the graph obtained by subdividing ij in G. If the graph energy of H is less than the graph energy of G, then one of the following two things is true.*

1. *The edge ij is the central edge in an induced diamond in G.*
2. *Let $W = \overline{N}(i)$. Then $\overline{N}(i) = \overline{N}(j) = W$ and $G[W]$ is a clique. Furthermore, each vertex in $W \setminus \{i, j\}$ has degree greater than i (i.e., each vertex in $W \setminus \{i, j\}$ is adjacent to at least one vertex outside of W in G).*

This conjecture is true for connected graphs up through 9 vertices. There are 2 connected graphs on 7 vertices which satisfy the hypotheses and not item 1. There are 23 connected graphs on 8 vertices and 261 connected graphs on 9 vertices which satisfy the hypotheses and not item 1. All of these graphs satisfy item 2. There are at least 1000 connected graphs on 10 vertices which satisfy the hypotheses and not item 1, but do satisfy item 2. Currently we are checking all connected graphs on 10 vertices.

A particularly interesting graph is the graph shown in Figure 2. This is the only graph on 8 or fewer vertices satisfying the hypotheses, but not item 1, such that subdividing two different edges decreases the energy.

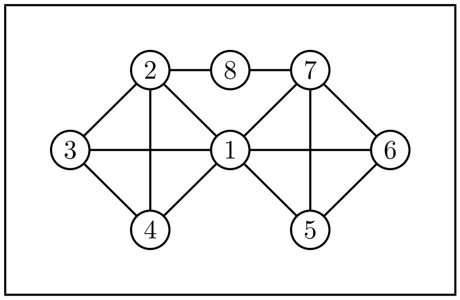

Figure 2: Subdividing 3—4 or 5—6 decreases the graph energy.

Conjecture 3.11. *If* q *is a prime power, then*

$$f(q+1) = \sqrt{q} + \frac{1}{q+\sqrt{q}+1}$$

Question 3.12. *Find* k*-regular graphs with high energy per vertex when* $k-1$ *is not a prime power.*

Question 3.13. *Determine all* 3*-regular bipartite graphs with* 5 *or* 6 *distinct eigenvalues.*

3.2 Laplacian energy

Let G be a connected graph with n vertices $\{1, 2, \ldots, n\}$ and degrees $d_1 \geq d_2 \geq \cdots \geq d_n \geq 1$ where $m = (d_1 + d_2 + \cdots + d_n)/2$ is the number of edges. Let $A(G) = A = [a_{ij}]$ be the adjacency matrix of G, and let D be the diagonal matrix of order n with diagonal entries $d_1, d_2, \ldots, d_n$. The matrix $L(G) = L = D - A$ (a singular M-matrix) is the Laplacian matrix of G and it has eigenvalues $\lambda_1 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$. The average degree of the vertices of G is $2m/n$ and

$$E_L(G) = E_L = \sum_{i=1}^{n} \left| \lambda_i - \frac{2m}{n} \right|$$

has been called the *Laplacian energy* of G.

Let $d = (d_1, d_2, \ldots, d_n)$ and $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$. Let $d^* = (d_1^*, d_2^*, \ldots, d_n^*)$ be the conjugate (degree) sequence of d. Then R. Grone and R. Merris[1] conjectured that λ is majorized by the conjugate of d, written $\lambda \preceq d^*$, that is,

$$\sum_{i=1}^{k} \lambda_i \leq \sum_{i=1}^{k} d_i^* \quad (k = 1, 2, \ldots, n)$$

with equality for $k = n$.

Since $|x - a|$ is a convex function of x, $\sum_{i=1}^{n} |x_{-}a_i|$ is also a convex function, and from majorization we conclude that **if** the Grone-Merris conjecture is true, then

$$E_L(G) \leq \sum_{i=1}^{n} \left| d_i^* - \frac{2m}{n} \right|.$$

There is a special class of graphs known as *threshold graphs*. These graphs admit a number of characterizations:

[1] *SIAM J. Discrete Math.*, 7 (2), 1994, 221–229.

1. Uniquely determined (as labelled graphs) by degree sequence.
2. Starting from one vertex, these are the graphs constructed recursively by adding an isolated or dominating (connected to all previous vertices) vertex.
3. The Laplacian eigenalues are $d_1^*, d_2^*, \ldots, d_n^*$.
4. $d_i = d_i^* - 1$ for all i with $1 \leq i \leq f_d$ where d is the largest k such that $d_k \geq k$ (the order of the so-called Durfee square in the Young diagram (Ferrers diagram) of d).[2]
5. With respect to the partial order of majorization, the degree sequence is maximal (no degree sequence of a graph properly majorizes the degree sequence of a threshold graph).

Note that a connected threshold graph must have a *dominating vertex* (a vertex connected to all the other vertices). Degree sequences of threshold graphs are called *threshold degree sequences.* The generating function for the number t_m of threshold graphs with m edges is

$$g(x) = \sum_{m \geq 0} t_m x^m = \prod_{i \geq 1} (1 + x^i),$$

the generating function for the number of strict partitions of m.. It is a known fact[3] that the extreme points of the convex hull of degree sequences of graphs with n vertices are precisely the degree sequences of threshold graphs.

The problems of focus were to determine the maximal Laplacian energy for

1. n (number of vertices) and m (number of edges) fixed.
2. n fixed but number m of edges not specified (possibly restricting to threshold graphs only).
3. m fixed, but number of vertices not specified (possibly restricting to threshold graphs only), and
4. What are the extreme points of the convex hull of the n-tuples $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ of of Laplacian eigenvalues of graphs with n vertices? (It was conjectured at first that these are the λ's for threshold graphs (so the conjugate degree vectors of threshold graphs) but this was shown to be false.)

At first it had been conjectured that the maximum Laplace energy was attained by *pineapples.* These are threshold graphs obtained by taking a complete graph K_p and adjoining $n - p$ other vertices and an edge from each of these vertices to one specified vertex of K_p; the degree sequence is then $n-1, p-1, \ldots, p-1, 1, \ldots, 1$ where there are $p-1$ degrees equal to $p-1$ and $n-p$ degrees equal to 1, and the conjugate degree sequence is $n, p, \ldots, p, 1, \ldots, 1, 0$ where there are $(p-2)$ p's and $(n-p)$ 1's. But a disconnected counterexample was found, still leaving the problem open for connected graphs.

Note that to maximize Laplacian energy, the Laplacian eigenvalues should be distributed in such a way to be far from their average $2m/n$.
Our discussion of these questions led to the following additional problems:

[2]See: The branching extent of graphs, E. Ruch and I. Gutman, *J. Combin, Inform. System Sci.*, 4, 1979, 285-295. Also see: R. Merris and T. Roby, The lattice of threshold graphs, *J. Inequal. Pure and Appl. Math.*, 6 (1), 2005, 1–20.

[3]See: N.V.R. Mahadev and U.N. Peled, *Threshold Graphs and Related Topics*, Annals Disc. Math., 56, North-Holland, Amsterdam, 1995.

(a) What is the maximum of

$$\sum_{i=1}^{n} \left| d_i^* - \frac{2m}{n} \right|.$$

over all graphs on n vertices and m edges?

(b) What is the maximum of

$$\sum_{i=1}^{n} \left| d_i^* - \frac{2m}{n} \right|.$$

over all graphs on n vertices and with m not specified?

(c) What are the extreme points of the convex hull of the conjugates of the degree sequences of graphs with n vertices? Characterize the graphs corresponding to the extreme points.

Concerning problem (a), it is not hard to show that the maximum occurs for regular graphs if they exist for given n and m (a regular graph of degree k has conjugate degree sequence equal to $n, \ldots, n, 0, \ldots, 0$ where there are k n's and $n - k$ 0's), otherwise the maximum occurs for a nearly regular graph. Concerning problem (b), the maximum for a regular graph of degree $\lfloor n/2 \rfloor$ or $\lceil n/2 \rceil$, or at a corresponding nearly-regular graph Problem (c), is under investigation, but the extreme points do not all correspond to regular or almost regular.

The following upper bound on $E_L(G)$ was obtained:

$$E_L(G) < 4m.$$