Algebraic and Extremal Graph Theory, University of Delaware

A Positive Proportion of Multigraphs Are Determined by Their Generalized Spectra

Wei Wang

Joint with Tao Yu

Xi'an Jiaotong University

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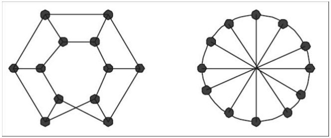
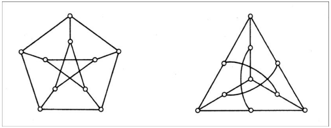
Outline

Introduction

Graph Isomorphism Problem (GIP)

Given two graphs G and H, determine whether they are isomorphic nor not.





A Recent Breakthrough

L. Babai (2015)

[a] There is a quasipolynomial time algorithm for all graphs, i.e., one with running time $\exp((\log n)^{O(1)})$.

[a] L. Babai, Graph isomorphism in quasipolynomial time, arXiv:1512.03547v2.

- It remains an unsolved question whether GIP is in $\mathcal{P}$ or in $\mathcal{NPC}$.

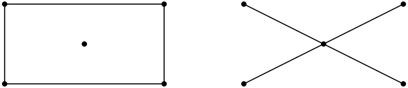
Graph Spectra and the Structures

- The spectrum of a graph encodes a lot of information about the given graph, e.g.,
- From the adjacency spectrum, one can deduce
  - (i) the number of vertices, the number of edges;
  - (ii) the number of triangles ;
  - (iii) the number of closed walks of any fixed length;
  - (iv) bipartiteness;

    ...
- From the Laplacian spectrum, one can deduce:
  - (i) the number of spanning trees;
  - (ii) the number of connected components;

    ...
- Can a graph be determined by its spectrum?

A pair of cospectral graphs



$$\begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

spectrum: -2, 0, 0, 0, 2

Which Graphs Are DS?

- "Which graphs are determined by spectrum(DS for short)?"
- In 1956, Günthard and Primas raised the question in a paper that relates the theory of graph spectra to Hückel's theory from chemistry.
- Applications:
  - Graph Isomorphism Problem;
  - The shape and sound of a drum;
  - Energy of hydrocarbon molecules;

  ....

Are Almost All Graphs DS?

- Are almost all graph DS? Are Almost all graphs non-DS? or Neither is true?

Conjecture (Haemers)

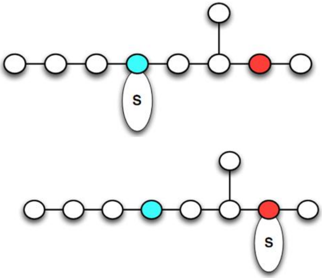
Almost all graphs are DS. [a]

[a] Formally speaking, the fraction of the DS graphs among all graphs tends to 1 as the order of the graphs tends to infinity.

The Conjecture is False for Trees

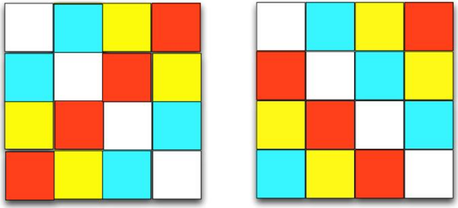
Schwenk (1973)

Almost every tree has a cospectral mate.



The Conjecture is False for Strongly Regular Graphs

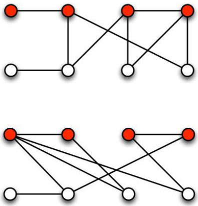
- 16 squares as vertices;
- adjacent if in same row, same column, or same color.
- The pair of strongly regular graphs constructed in this way are cospectral.
- There are lots of Latin squares.



Cospectral and Non-isomorphic Graphs Can Easily Be Constructed

Godsil and McKay (1982), GM-switching

Let the vertex set V of G can be partitioned into V and V_2. Suppose $G[V_1]$ is regular, and every vertex in V_2 is adjacent to non, all, or exactly half number of vertices in V_1. Then the new graph obtained by GM-switching and the old one are cospectral.



Very Few Graphs Are Known to Be DS

1. The complete graph K_n.
2. The regular complete bipartite graph $K_{n,n}$.
3. The cycle C_n.
4. The path P_n.
5. The tree Z_n.
6. $\cdots\cdots\cdots$

Computer Enumerations

Table: Fractions of DS Graphs

n	# Graphs	Fraction	References
2	2	1	
3	4	1	
4	11	1	
5	34	0.941	
6	156	0.936	
7	1044	0.895	
8	12346	0.861	
9	274668	0.814	Godsil, McKay (1982)
10	12005168	0.787	Haemers, Spence (2004)
11	1018997864	0.792	Haemers, Spence (2004)
12	165091172592	0.812	Brouwer, Spence (2009)

A Recent Result

- A graph G is determined by its generalized spectrum (DGS for short), if for any graph H, H and G are cospectral with cospectral complements implies that H isomorphic to G.
- Let G be a graph with adjacency matrix A. Define $W = [e, Ae, \cdots, A^{n-1}e]$ (e is the all-one vector).

Theorem [Wang, 2017]

If $\frac{\det(W)}{2^{\lfloor n/2 \rfloor}}$ (which is always an integer) is odd and square-free, then G is DGS.

- W. Wang, A simple arithmetic criterion for graphs being determined by their generalized spectra, JCTB, 122 (2017) 438-451.

What is the density of $\mathcal{F}_n$?

- $\mathcal{F}_n := \{G \mid \det(W)/2^{\lceil n/2 \rceil} \text{ is odd and square} - \text{free}\}$.

Table: Fractions of Graphs in $\mathcal{F}_n$

n	The Fractions
10	0.211
15	0.201
20	0.213
25	0.216
30	0.233
35	0.229
40	0.198
45	0.202
50	0.204

- The above numerical results suggest that $\mathcal{F}_n$ may have positive density. This gives strong evidence for Haemers' conjecture.

The Main Results

1. We gave a simple and efficient condition for a multigraph to be DGS.
2. Based on this, we showed that a family of multi-graphs $\mathcal{D}_n$ are DGS, and derived a close formula for the density of $\mathcal{D}_n$, i.e.,

$$\mu(\mathcal{D}_n) = \Pi_p(1 - \frac{c_p}{p^d}),$$

where p runs over all primes, $d = (n+1)n/2$, and

$$c_p = \#\{A \in S_n(\mathbb{F}_p) | \Delta(A) = \Delta(A+J) = 0\}.$$

(Remark: The ratio c_p/p^d is the probability that a matrix $A \in S_n(\mathbb{F}_p)$ has the following property: both the characteristic polynomials of A and $A+J$ have multiple factors over $\mathbb{F}_p$.)

3. We showed $\mu(\mathcal{D}_n) > 0$ for every n. We further conjectured that $\mu(\mathcal{D}_n) \to c_0 \approx 0.22$, as n goes to infinity.

Notations and Terminologies

- Define $\mathrm{Box} = \{(a_1, a_2, \cdots, a_d) \in \mathbb{Z}^d | 0 \leq a_i \leq b\}$, for $b > 0$.
- The density of a set $S \subset \mathbb{Z}^n$ is defined as

$$\mu(S) = \lim_{b\to\infty} \frac{\#(S \cap Box)}{\#(Box)}.$$

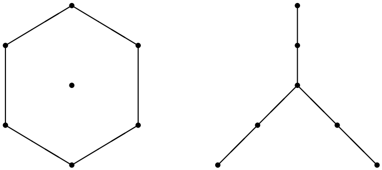
- Let $\mathcal{S}_n$ be a subset of all multigraphs of order n.
- The adjacency matrix $A(G) = (a_{ij})$ can be identified as a vector in $\mathbb{Z}^d$ ($d = \frac{n(n+1)}{2}$). So $\mathcal{S}_n$ has a natural density $\mu(\mathcal{S}_n)$.

Notations and Terminologies -cont'd

- $G = (V, E)$: a multi-graph
  vertex set: $V = \{v_1, v_2, \ldots, v_n\}$;
  edge set: $E = \{e_1, e_2, \ldots, e_m\}$.
- *The adjacency matrix* $A(G) = (a_{ij})$ of G is a matrix with $a_{ij} = \text{the number of edges between } v_i \text{ and } v_j$.
- *The characteristic polynomial of* G is defined as $\phi(G; \lambda) = \det(\lambda I - A(G))$.
- *The spectrum* of G, denoted by $\mathrm{Spec}(G)$, is the multiset of all the eigenvalues of $A(G)$.
- Two multi-graphs G, H are *cospectral* if $\mathrm{Spec}(G) = \mathrm{Spec}(H)$.
- $\mathbb{F}_p$ denotes a finite field with p elements (p is a prime number), $\mathbb{Z}$ ($\mathbb{Z}^+$) denotes the set of (nonnegative) integers.

Notations and Terminologies - cont'd.

- Two (multi)-graphs G and H are *cospectral w.r.t. the generalized spectrum* if $\mathrm{Spec}(G) = \mathrm{Spec}(H)$ and $\mathrm{Spec}(\bar{G}) = \mathrm{Spec}(\bar{H})$.
- E.g.



$$P_{G_1}(\lambda) = P_{G_2}(\lambda) = \lambda^7 - 6\lambda^5 + 9\lambda^3 - 4\lambda$$

$$P_{\bar{G}_1}(\lambda) = P_{\bar{G}_2}(\lambda) = \lambda^7 - 15\lambda^5 - 2\lambda^4 + 12\lambda^3 + 24\lambda^2$$

DGS Graphs

- A multi-graph G is said to be determined by the generalized spectrum (DGS for short), if any multi-graph that is cospectral with G w.r.t. the generalized spectrum is isomorphic to G.
- In notation, G is DGS if $\mathrm{Spec}(G) = \mathrm{Spec}(H)$ and $\mathrm{Spec}(\bar{G}) = \mathrm{Spec}(\bar{H})$ implies H is isomorphic to G for any H.

Walk-matrix

The walk-matrix of multi-graph G:

$$W(G) = [e, A(G)e, \ldots, A(G)^{n-1}e]$$

where $e = (1, 1, \ldots, 1)^T$ is the all-one vector.

- The (i, j)-th entry of W is the number of walks of length $j - 1$ starting from the i-th vertex.

Controllable Multi-Graphs

- A multi-graph G is called controllable if the corresponding walk-matrix $W(G)$ is non-singular.
- For controllable graphs, it was conjectured (by C.D. Godsil) that almost all graphs are controllable. O$'$Rourke and Touri showed recently that this conjecture is true.

A Simple Characterization

Theorem [C.f. Wang and Xu, 2006]

Let G be a controllable (multi)-graph. Then there exists a (multi)-graph H such that $\mathrm{Spec}(G) = \mathrm{Spec}(H)$ and $\mathrm{Spec}(\bar{G}) = \mathrm{Spec}(\bar{H})$ if and only if there exists a unique rational orthogonal matrix Q such that

$$Q^T A(G) Q = A(H), \text{ and } Qe = e, \tag{1}$$

where e is the all-ones vector.

How to Find DGS-Graphs?

- $O_n(\mathbb{Q})$: the set of all rational orthogonal matrices.
- $S_n(\mathbb{Z}^+)$: the set of symmetric matrices with all the entries being non-negative integers.

Definition

$\Gamma(G) = \{Q \in O_n(\mathbb{Q}) | Q^T A(G) Q \in S_n(\mathbb{Z}^+) \text{ and } Qe = e\}.$

Theorem [C.f. Wang and Xu, 2006]

Let G be a controllable multi-graph. Then G is DGS if and only if $\Gamma(G)$ contains only permutation matrices.

- Question: How to find out all $Q \in \Gamma(G)$ explicitly?

The Level of Q

Definition

Let Q be a rational orthogonal matrix with $Qe = e$, the level of Q is the smallest positive integer ℓ such that ℓQ is an integral matrix.

- The matrix Q is a permutation matrix if and only if $\ell = 1$.
- Example:

$$\frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}, \frac{1}{3}\begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ -1 & 2 & -1 & 1 & 1 & 1 \\ -1 & -1 & 2 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & -1 & -1 \\ 1 & 1 & 1 & -1 & 2 & -1 \\ 1 & 1 & 1 & -1 & -1 & 2 \end{bmatrix}.$$

The Discriminant of a Matrix

- Let $f(x) \in \mathbb{Z}[x]$ be a polynomial, the discriminant of f is defined as $\Delta(f) := \Pi_{i<j}(\lambda_i - \lambda_j)^2$, where λ_i are the roots of f over $\mathbb{C}$.
  E.g. $f(x) = ax^2 + bx + c$, $\Delta(f) = b^2 - 4ac$.
- The discriminant of a matrix M, denoted by $\Delta(M)$, is defined to be the discriminant of its characteristic polynomial.
- The discriminant of a multigraph G, denoted by $\Delta(G)$ or $\Delta(A_G)$, is defined to be that of its adjacency matrix.
- Clearly, $\Delta(A_G)$ is an integer for any multigraph G.

A New Arithmetic Criterion

- Define $\Gamma(G) = \{Q \in O_n(\mathbb{Q}) | Q^T A(G) Q \in S_n(\mathbb{Z}^+), Qe = e\}$.

Theorem [Wang and Yu, 2017]

Let G be a multigraph with adjacency matrix A_G, and J the all-ones matrix. Let $d(G) := \gcd\{\Delta(A_G + tJ)) | t \in \mathbb{Z}\}$. If $d(G)$ is odd and square-free, then $\Gamma(G)$ contains only permutation matrices and G is DGS.

Corollary

If $\gcd(\Delta(A_G), \Delta(A_G + J)) = 1$, *then* G *is DGS.*

- W. Wang, T. Yu, A positive proportion of multigraphs are determined by their generalized spectra, manuscript, 2017.

The Key Ingredient

Lemma

Let G be a multigraph with adjacency matrix A_G. Let $Q \in \Gamma(G)$ with level $\ell \neq 1$. Let p be any prime divisor of ℓ. Then $p \mid \Delta(A_G)$.

Lemma

Let G be a multigraph with adjacency matrix A_G. Let $Q \in \Gamma(G)$ with level $\ell \neq 1$. Let $p > 2$ be any prime divisor of ℓ. Then $p^2 \mid \Delta(A_G)$.

Proof of the Corollary

- From $Q \in \Gamma(G)$ we know $Q^T A_G Q = A_H$ for some multigraph H. It follows that $Q^T(A_G + tJ)Q = A_H + tJ$ for any $t \in \mathbb{Z}$. Thus, $p \mid \Delta(A_G + tJ)$, $\forall t \in \mathbb{Z}$.
- If $\gcd\{\Delta(A_G + tJ) | t \in \mathbb{Z}\} = 1$, then G is DGS. In particular, if $\gcd(\Delta(A_G), \Delta(A_G + J)) = 1$, then G is DGS.
- The Corollary provides us an efficient method to test whether G is DGS. More importantly, it provides us a way to show that the set of DGS-multigraphs has positive density!

Another Ingredient

Theorem [Pooen, 2003]

Let $f, g \in \mathbb{Z}[x_1, x_2, \cdots, x_d]$ be two polynomials that are relatively prime as elements of $\mathbb{Z}[x_1, x_2, \cdots, x_d]$. Let

$$\mathcal{R} = \{a \in \mathbb{Z}^d \,|\, \gcd(f(a), g(a)) = 1\}.$$

Then $\mu(\mathcal{R}) = \Pi_p(1 - \frac{c_p}{p^d})$, where

$$c_p = \#\{x \in \mathbb{F}_p^d | f(x) = g(x) = 0 \text{ over } \mathbb{F}_p\}.$$

- B. Poonen, Square-free values of multivariate polynomials, Duke Math. Journal, 118 (2003) 353-373.

Applying Poonen's Theorem to Our Case

- Let $X = (x_{ij})_{n\times n}$ $(x_{ij} = x_{ji})$ be the adjacency matrix of a multi-graph, where x_{ij} are intermediates.
- Then $\Delta(X)$ is a multivariate polynomial in the ring $\mathbb{Z}[x_{11}, x_{12}, \cdots, x_{nn}]$.
- We can show

Theorem [Wang and Yu, 2017]

The multivariate polynomial $\Delta(X)$ is irreducible in $\mathbb{Z}[x_{11}, x_{12}, \cdots, x_{nn}]$.

Corollary

$\Delta(X)$ and $\Delta(X + J)$ are relatively prime in $\mathbb{Z}[x_{11}, x_{12}, \cdots, x_{nn}]$.

Applying Poonen's Theorem to Our Case

- $\mathcal{D}_n := \{A \in S_n(\mathbb{Z}^+) | \Delta(A) = \Delta(A+J) = 0, \det(W(A)) \neq 0\}$ and $\bar{\mathcal{D}}_n := \{A \in S_n(\mathbb{Z}^+) | \Delta(A) = \Delta(A+J) = 0\}$. Then $\mu(\mathcal{D}_n) = \mu(\bar{\mathcal{D}}_n)$.
- $\bar{\mathcal{D}}_n = \{(x_{11}, \cdots, x_{nn}) \in \mathbb{Z}^d | \gcd(\Delta(X), \Delta(X+J)) = 1\}$. Then

$$\mu(\mathcal{D}_n) = \mu(\bar{\mathcal{D}}_n) = \Pi_p(1 - \frac{c_p}{p^d}),$$

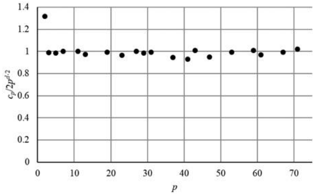
  where $c_p = \#\{x \in \mathbb{F}_p^d | \Delta(X) = \Delta(X+J) = 0 \text{ over } \mathbb{F}_p\}$, and $d = \frac{n(n+1)}{2}$.
- We are able to show $1 - \frac{c_p}{p^d} > 0$ for any p;
- Moreover, $c_p/p^d = O(1/p^2)$ (the Lang-Weil bound).
- Thus the infinite product converges and $\mu(\mathcal{D}_n) > 0$ for any fixed n.

The estimates of c_p/p^d

Conjecture 1

$$\lim_{n\to\infty}\frac{c_p}{p^d}=\begin{cases}\rho_2\approx 0.65, \text{for } p=2;\\ 2/p^2, \text{for } p>2.\end{cases}$$

- If the above conjecture is true, then $\lim_{n\to\infty}\mu(\mathcal{D}_n)=(1-\rho_2)\prod_{p>2}(1-\frac{2}{p^2})\approx 0.22.$



What is the density $\mu(\mathcal{D}_n)$?

- $\mathcal{D}_{n,b}$: the subset of $\mathcal{D}_n$, in which every multi-graph has at most b edges between any two vertices.

Table: Density of $\mu(\mathcal{D}_{n,b})$

n	$b=1$	$b=10$	$b=10^2$	$b=10^3$	$b=10^4$
5	0.2733	0.2364	0.2357	0.2313	0.2318
10	0.2342	0.2210	0.2162	0.2197	0.2213
20	0.2225	0.2229	0.2261	0.2257	0.2327
30	0.2227	0.2175	0.2213	0.2209	0.2178
40	0.2239	0.2240	0.2160	0.2219	0.2214
50	0.2250	0.2197	0.2298	0.2250	0.2223
60	0.2220	0.2198	0.2269	0.2274	0.2198
70	0.2198	0.2259	0.2237	0.2260	*
80	0.2229	0.2253	0.2201	*	*

- The data was obtained by randomly generated 10,000 graphs independently at each time, then count the number of DGS graphs among them.

Another Conjecture

- $\mathcal{D}_{n,b}$: the subset of $\mathcal{D}_n$, in which every multi-graph has at most b edges between any two vertices.

Conjecture 2

The density $\lim_{n\to\infty} \mu(\mathcal{D}_{n,b})$ is independent of b.

- If the above conjecture were true, then we would be very close to the statement "DGS graphs has positive density".

Conclusions

1. We have shown that the set of all multigraphs on n vertices that are DGS has a positive density for every fixed n.
2. We guess there is a uniform lower bound for the density for every n (around 0.22); maybe this is not difficult.
3. This gives strong evidence for Haemers' conjecture that "Almost All Graphs Are DS".
4. However, for simple graphs, we still don't know the answer; for other kind of spectrum (of adjacency matrices, Laplacian matrix, etc), we don't know the answer either.
5. There are still more to be investigated in the future!

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Thank you!
The end!

The r-complement of a multi-graph

- G: a multigraph with adjacency matrix A. Let r be a non-negative integer large enough. The r-complement of G is a multigraph with adjacency matrix $rJ - A$, denoted by $\bar{G}_r$. Two multigraphs are generalized r-cospectral if $\mathrm{Spec}(G) = \mathrm{Spec}(H)$ and $\mathrm{Spec}(\bar{G}_r) = \mathrm{Spec}(\bar{H}_r)$ for some r.
- This definition is independent of r.

$$\phi(x) = x^4 - 3x^3 - 27x^2 + 18x + 36,$$

$$\bar{\phi}(x) = \phi(-x) + r(-4x^3 + 13x^2 + 18x - 18),$$