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The structure of graphs with small M-indices

Joint research with E.M. Li Marzi, S.K. Simić and J. Wang

Notation

Let M ($= M(G)$) be a graph matrix associated to some graph G. The characteristic polynomial of M (i.e. $\det(xI - M)$) is called the *M-polynomial of G*. The eigenvalues of M, namely the zeros of the M-polynomial, and its spectrum (which consists of the n M-eigenvalues) are called the *M-eigenvalues* and *M-spectrum* of G, respectively. The largest eigenvalue of G is called the *M-index*.

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In this talk M will be one of the following matrices:

- A, the adjacency matrix;
- $L = D - A$, the Laplacian matrix, where D is the diagonal matrix of vertex degrees.
- $Q = D + A$, the signless Laplacian.

Notation

The following notation will be used in the rest:

A-theory: $\phi(G,x)$ is the A-polynomial, $\rho(G)$ is the A-index;

L-theory: $\psi(G,x)$ is the L-polynomial, $\mu(G)$ is the L-index;

Q-theory: $\varphi(G,x)$ is the Q-polynomial, $\kappa(G)$ is the Q-index;

We will now shortly survey some important results which link the above polynomials and their corresponding theories.

Theorem

Let G be a graph. Then $\psi(G) = \varphi(G)$ if and only if G is bipartite. If G is non bipartite then $\mu(G) < \kappa(G)$.

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Theorem

Let G be a graph of order n and size m, and let $S(G)$ be the subdivision graph of G. Then

$$\phi(S(G), x) = x^{m-n}\varphi(G, x^2).$$

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The above results can be seen as *bridges* among the above theories. So a result given for the A-theory can be *translated* to the Q-theory and then to the L-theory, and vice versa.

The graphs mentioned in this talk are: the path P_n, the cycle C_n, the lollipop L_g^p, consisting of a cycle of lenght g with a pendant path of lenght p. Here are depicted some other graphs.

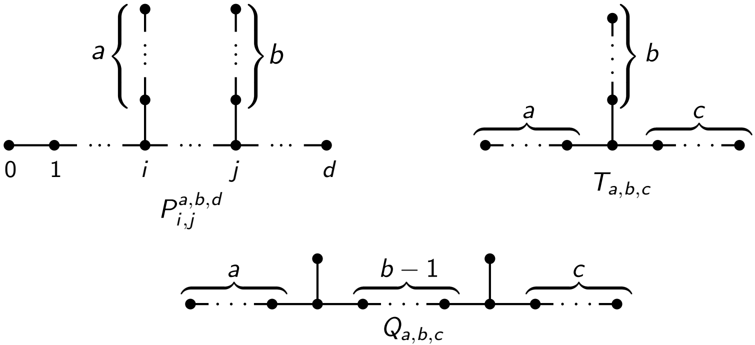

Fig. 1: Graphs $P_{i,j}^{a,b,d}$, $Q_{a,b,c}$ and $T_{a,b,c}$.

Hoffman limit values

We will consider the (connected) graphs whose M-index, $M \in \{A, L, Q\}$, does not exceed the limit point for the M-index of the *Hoffman graph* H_n, that is a cycle on $n-1$ vertices with a pendant edge ($H_n = L^1_{n-1}$). The latter limit point will be called the *M-Hoffman limit value*:

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A-Hoffman l. v.: $\lim_{n\to\infty} \rho(H_n) = \sqrt{2+\sqrt{5}}$; (Hoffman, 1972)

L-Hoffman l. v.: $\lim_{n\to\infty} \mu(H_n) = 2+\epsilon$; (Guo, 2008)

Q-Hoffman l. v.: $\lim_{n\to\infty} \rho(H_n) = 2+\epsilon$; (Wang et al., 2009)

where $2+\epsilon$ is the real root of $x^3 - 6x^2 + 8x - 4$.

The Hoffman program

Hoffman was the first who considered graph limit points for the graph eigenvalues and he found many limit values. In particular he found all limit points between 2 and $\sqrt{2+\sqrt{5}}$. Shearer later proved that all real values greater than $\sqrt{2+\sqrt{5}}$ are limit points for the A-index of some sequence of graphs (in particular, caterpillars). One question arose at that time:

"Which are the graphs whose A-index do not exceed the (A-)Hoffman limit value?"

The latter is the *Hoffman program* (for the A-theory).

Graphs whose A-index does not exceed 2

In 1972, Smith determined all connected graphs whose A-index is exactly 2, those graphs nowadays are known as the *Smith graphs*. By the Interlacing Theorem, we also know that their proper subgraphs are those whose A-index is less than 2.

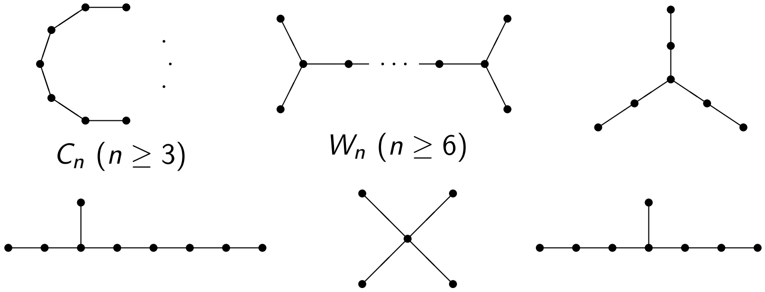

Fig. 2: Smith graphs.

Let $\mathcal{G}_M(\lambda)$ be the set of connected graphs whose M-index does not exceed λ. The Hoffman program for the A-theory, i.e. the complete determination of the set $\mathcal{G}_A(\sqrt{2+\sqrt{5}})$, was considered by several authors. Cvektović et al. determined the structure of the graphs in $\mathcal{G}_A(\sqrt{2+\sqrt{5}})$...

Theorem (Cvetoković, Doob, Gutman, 1986)

$\mathcal{G}_A(\sqrt{2+\sqrt{5}}) = \mathcal{G}_A(2) \cup \{\, T_{a,b,c} \mid a=1, b=2, c>5;\ \text{or } a=1, b>2, c>3;\ \text{or } a=b=2, c>2;\ \text{or } a=2, b=c=3\} \cup \{\, Q_{a,b,c} \mid (a,b,c) \in \mathcal{S};\ \text{or } c \geq a > 0, b \geq b^*(a,c), (a,c) \neq (1,1)\}$,

where $\mathcal{S} = \{(1,1,2),(2,4,2),(2,5,3),(3,7,3),(3,8,4)\}$ *and* $b^*(a,c)$ *is an integer function.*

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... and Brouwer and Neumaier finally completed the investigation:

Theorem (Brouwer, Neumaier, 1989)

$\mathcal{G}_A(\sqrt{2+\sqrt{5}}) = \mathcal{G}_A(2) \cup \{T_{a,b,c} \mid a=1, b=2, c>5;\ \text{or } a=1, b>2, c>3;\ \text{or } a=b=2, c>2;\ \text{or } a=2, b=c=3\} \cup \{Q_{a,b,c} \mid (a,b,c) \in \mathcal{S};\ \text{or } c \geq a > 0, b \geq b^*(a,c), (a,c) \neq (1,1)\}$, *where* $\mathcal{S} = \{(1,1,2),(2,4,2),(2,5,3),(3,7,3),(3,8,4)\}$ *and*

$$b^*(a,c) = \begin{cases} a+c+2, & \text{for } a>2; \\ c+3, & \text{for } a=2; \\ c, & \text{for } a=1. \end{cases}$$

What about the other spectra?

About the other spectra, the whole story developed completely just recently:

In 2008, Guo computed the L-Hoffman limit value, that is $2+\epsilon \approx 4.38$, the real root of $x^3 - 6x^2 + 4x - 8$. Also Guo determined all limit points between 4 and $2+\epsilon$, and the latter result is the L-variant of the original result of Hoffman for the A-theory. What about the (connected) graphs whose L-index does not exceed $2+\epsilon$?

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In fact the problem seems to be difficult. Maybe solving it for the Q-theory might help... so Wang et al. started the study for the Hoffman program in the Q-theory.

The graphs whose Q-index does not exceed 4 were determined by Cvetković et al. in 2006/7. But nothing else was done w.r.t. the Q-theory, so Wang et al. reproduced the result of Guo on the L-theory for the Q-theory. In fact, all limit points for the Q-index between 4 and $2+\epsilon$ are indeed the same as those for the L-theory.

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The smallest Q-limit point after 4 is $2+\sqrt{5}$, so it is natural to consider first $\mathcal{G}_Q(2+\sqrt{5})$. A graph in latter set must be a tree with just one vertex of degree 3. Indeed, any unicyclic graph - different from a cycle - has its Q-index larger than some Hoffman graph (by the Hoffman-Smith lemma on internal paths), hence its Q-index exceeds $2+\epsilon$; in addition, $\kappa(W_n), \kappa(T_{1,2,2}) > 2+\sqrt{5}$.

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Theorem

[Cvektović et al., 2007] $\mathcal{G}_Q(4) = \{P_n, C_n, K_{1,3}\}$

[Wang et al., 2009] $\mathcal{G}_Q(2+\sqrt{5}) = \mathcal{G}_Q(4) \cup \{T_{1,1,a}, a \geq 2\}$.

Wang et al. also proved that the graphs in $\mathcal{G}_Q(2+\epsilon) \setminus \mathcal{G}_Q(2+\sqrt{5})$ must be trees with just two vertices of degree 3, in particular:

Theorem (Wang, Huang, Belardo, Li Marzi, 2009)

$\mathcal{G}_Q(2+\epsilon) = \mathcal{G}_Q(2+\sqrt{5}) \cup \{Q_{a,b^*(a,c),c}\}$,
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$\mathcal{G}_Q(2+\epsilon) = \mathcal{G}_Q(2+\sqrt{5}) \cup \{Q_{a,b^*(a,c),c}\}$, where $b^*(a,c)$ is an integer function.

The authors also gave the following conjecture:

Conjecture

$\kappa(Q_{a,b,c}) < 2+\epsilon$ if and only if $b \geq a+c+1$.

The above conjecture was solved just recently, thanks to the A-theory.

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First step: Simplify the conjecture.
Indeed, it was possible to prove that

$$\kappa(Q_{1,k,k-1}) > 2+\epsilon \;\text{ implies }\; \kappa(Q_{a,b,c}) > 2+\epsilon \;\text{ when }\; b < a+c+1$$

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Second step: Translate to the A-theory. Indeed from $S(Q_{1,k,k-1}) = P^{2,2,4k}_{2,2k+2}$, we can deduce

$$\rho(P^{2,2,4k}_{1,2k+1}) > \sqrt{2+\epsilon} \quad \text{implies} \quad \kappa(Q_{1,k,k-1}) > 2+\epsilon.$$

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Third step: Prove that $\phi(P^{2,2,4k}_{1,2k+1}), \sqrt{2+\epsilon}) < 0$.

$\rho(G_k) > \sqrt{2+\epsilon}$

To simplify the notation let $G_k = P^{2,2,4k}_{1,2k+1}$. In order to check that $\phi(G_k, \sqrt{2+\epsilon}) < 0$, we need to compute explicitly the characteristic polynomial of G_k. Recently Ramezani et al. showed that

$$\phi(P_m, \lambda) = \frac{x^{2m+2} - 1}{x^{m+2} - x^m},$$

where where x satisfies $x^2 - \lambda x + 1 = 0$.

So if we express the polynomial of G_k in terms of paths, we get:

$$\begin{aligned}\phi(G_k, \lambda) &= \lambda\phi(T_{2,2k-1,2k+2}) - (\lambda^2 - 1)\phi(T_{2,2k-1,2k-1}) \\ &= \lambda[(\lambda^2 - 1)\phi(P_{4k+2}) - \lambda\phi(P_{2k+2})\phi(P_{2k-1})] \\ &\quad -(\lambda^2 - 1)[(\lambda^2 - 1)\phi(P_{4k-1}) - \lambda\phi^2(P_{2k-1})].\end{aligned}$$

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So if we express the polynomial of G_k in terms of paths, we get:

$$\begin{aligned}\Phi(G_k, x) \quad = \quad & [x^{8k+2}(x^{12} - x^{10} - 2x^8 - x^6 + 2x^4 + 2x^2 + 1) \\ & +x^{4k+2}(x^{10} - 3x^6 - 3x^4 + 1) + (x^{12} + 2x^{10} \\ & +2x^8 - x^6 - 2x^4 - x^2 + 1)] \cdot [x^{4k+5}(x^2 - 1)^2]^{-1}.\end{aligned}$$

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So we have that

$$\phi(G_k, \sqrt{2+\epsilon}) < 0 \quad \text{iff} \quad \Phi(G_k, \epsilon') < 0,$$

where $\epsilon' = (\sqrt{\epsilon+2} + \sqrt{\epsilon-2})/2$.

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where $\epsilon' = (\sqrt{\epsilon+2} + \sqrt{\epsilon-2})/2$.

The latter inequality was proved to be true and consequently the following theorem was given:

Theorem (Belardo, Li Marzi, Simić, Wang, 2010)
$\kappa(Q_{a,b,c}) > 2+\epsilon \quad \text{if and only if} \quad b < a+c+1.$

Hoffman program for the Q-theory

So the Q-Hoffman program is finally completed.

Theorem

Let $\mathcal{G}_Q(\kappa)$ be the set of connected graphs whose Q-index does not exceed κ. Then

- $\mathcal{G}_Q(4) = \{P_n, C_n, K_{1,3}\}$;
- $\mathcal{G}_Q(2+\sqrt{5}) = \mathcal{G}_Q(4) \cup \{T_{1,1,n-3}\,(n \geq 5)\}$;
- $\mathcal{G}_Q(2+\epsilon) = \mathcal{G}_Q(2+\sqrt{5}) \cup \{T_{1,b,c}\,(c \geq b \geq 2), Q_{a,b,c}\,(b \geq a+c+1)\}$.

Hoffman program for the L-theory

What we can say about the Hoffman program for the L-theory?

Recall that for bipartite graphs the L-polynomial and Q-polynomial are the same. The graphs in $\mathcal{G}_Q(2+\epsilon)$ are trees (so bipartite graphs). Hence to complete the Hoffman program for the L-theory, we need only to consider the non bipartite graphs.

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The following result of Guo is very useful in this context:

Theorem (Guo, 2007)

Let v be a vertex in a connected graph G and suppose that at v there are $s \geq 2$ hanging paths of equal length. If $\Delta(G) \geq s+1$, then adding any edge between vertices of degree 1 in the above hanging paths does not increase the L-index.

Hoffman program for the L-theory

Hence, by combining the results from the Q-theory, by using the latter result of Guo and by discarding other graphs (by using a forbidden subgraphs argument), we are able to state the following theorem which completes the Hoffman program for the L-theory (in blue you have the non-bipartite graphs):

Theorem (Wang, Belardo, Huang, Li Marzi, 2010)

Let $\mathcal{G}_L(\mu)$ be the set of connected graphs whose L-index does not exceed μ. Then

- $\mathcal{G}_L(4) = \{P_n, C_n, K_{1,3}, K_4, K_4^-, K_{1,3}^+\}$;
- $\mathcal{G}_L(2+\sqrt{5}) = \mathcal{G}_L(4) \cup \{T_{1,1,n-3}\,(n \geq 5), L_3^{n-3}\,(n \geq 5)\}$;
- $\mathcal{G}_L(2+\epsilon) = \mathcal{G}_L(2+\sqrt{5}) \cup \{Q_1, Q_2, T_{1,b,c}\,(c \geq b \geq 2), L_{2k+1}^1\,(k > 1), W_n, D_n^-, D_n\,(n \geq 8), Q_{a,b,c}\,(b \geq a+c+1)\}$.

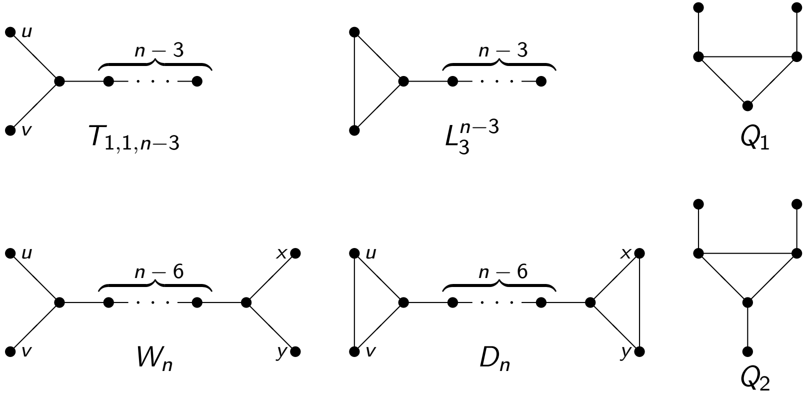

Fig. 3: Some graphs in $\mathcal{G}_L(2+\epsilon)$.

Other relevant limit values

The following theorem is due to Hoffman and Smith (1975):

Theorem

Let $G = G_0$ be a graph with maximum vertex degree Δ, and let G_n be $S(G_{n-1})$ then

$$\lim_{n\to\infty} \rho(G_n) = \frac{\Delta}{\sqrt{\Delta - 1}} = \mathrm{Hoff}_A(\Delta).$$

For the $\{L, Q\}$-theory similarly we have

Theorem

Let $G = G_0$ be a graph with maximum vertex degree Δ, and let G_n be $S(G_{n-1})$ then

$$\lim_{n\to\infty} \kappa(G_n) = \frac{\Delta^2}{\Delta - 1} = \mathrm{Hoff}_Q(\Delta).$$

Extended Hoffman program

If $\Delta = 3$ we get the following limit value (which naturally appeared in different contexts):

$$\mathrm{Hoff}_A(3) = 3\frac{\sqrt{2}}{2}.$$

The above value has already been considered by several authors (for example, Brouwer and Neumaier, Cioaba et al., Wang et al.). However the set $\mathcal{G}_A(3\frac{\sqrt{2}}{2})$ is not (yet) completely characterized.

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Open Problem: *Describe the set* $\mathcal{G}_A(3\frac{\sqrt{2}}{2})$.

The similar problem can be consider for the other two theories (note, $(3\frac{\sqrt{2}}{2})^2 = 4.5$):

Open Problem: *Describe the sets* $\mathcal{G}_Q(4.5)$ *and* $\mathcal{G}_L(4.5)$.

Thank you!!

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The structure of graphs with small M-indices

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