Unified extremal results of topological index and graph spectrum

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(Jointed work with **Muhuo Liu, Francesco Belardo, Chao Yang**)

[Y. Yao, M. Liu, F. Belardo, C. Yang, DAM, on line]

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Background and Definitions

- As usual, denote $d(u)$ the degree of u, denote $dist(u, v)$ the distance between u and v.

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- Suppose the degree of vertex v_i equals d_i for $i = 1, 2, \ldots, n$, then $\pi(G) = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G.
- Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π.

- The **first Zagreb index** $M_1(G)$ and **second Zagreb index** $M_2(G)$ [I. Gutman, N. Trinajstić, *Chem. Phys. Lett.*, 1972.]:

$$M_1(G) = \sum_{v \in V(G)} d^2(u), \quad and \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

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- Došlić [*Ars Math. Contemp.*, 2008] defined the **first Zagreb coindex** $\overline{M_1(G)}$ and **second Zagreb coindex** $\overline{M_2(G)}$ of G as follows:

$$\overline{M_1(G)} = \sum_{uv \notin E(G)} (d(u) + d(v)), \qquad \overline{M_2(G)} = \sum_{uv \notin E(G)} d(u)d(v).$$

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- The following two topological indices are called the **multiplicative Zagreb indices** of G, and they were constructed by Todeschini et al. in 2010 [R. Todeschini, V. Consonni, *MATCH Commun. Math. Comput. Chem.*, 2010]:

$$\prod_1(G) = \prod_{u \in V(G)} d^2(u), \text{ and } \prod_2(G) = \prod_{u \in V(G)} (d(u))^{d(u)}.$$

- We define $\prod^{q}(G)$ as follows:

$$\prod^{q}(G)=\prod_{u\in V(G)}\left(d(u)\right)^{q}\Longrightarrow \ln\left(\prod^{q}(G)\right)=\sum_{v\in V(G)} q\ln\left(d(u)\right).$$

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- Let $f(x)$ be a function defined on positive real number. To unified the research of topological index defined on the degree of a graph G, we establish the notation of $H_f(G)$ associated with $f(x)$, where

$$H_f(G) = \sum_{v\in V(G)} f\left(d(v)\right).$$

Background and Definitions

- The **general sum-connectivity index** $\chi_q(G)$ of G is constructed as [B. Zhou, N. Trinajstić, *J. Math. Chem.*, 2010.]

$$\chi_q(G) = \sum_{uv \in E(G)} (d(u) + d(v))^q .$$

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$$\chi_q(G) = \sum_{uv \in E(G)} (d(u) + d(v))^q .$$

- The **reformulated Zagreb index** $Z_2(G)$ of G is defined as [A. Miličević, S. Nikolić, N. Trinajstić, *Mol. Diversity.*, 2004.]:

$$Z_2(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 .$$

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- As an extension of $Z_2(G)$, we define $Z_q(G)$ as follows:

$$Z_q(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^q .$$

Definition [H. Wang, *Cent. Eur. J. Math.*, 2014.]:

To unify these vertex-degree-based invariants, H. Wang defined **connectivity function** of a connected graph G associated with a symmetric bivariate function $\varphi(x, y)$ as

$$M_{\varphi}(G) = \sum_{uv \in E(G)} \varphi\big(d(u), d(v)\big). \tag{1}$$

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$$M_{\varphi}(G) = \sum_{uv \in E(G)} \varphi\big(d(u), d(v)\big). \tag{1}$$

- (i) $\varphi(x, y) = (x + y)^q \Longrightarrow M_{\varphi}(G) = \chi_q(G)$.

  (ii) $\varphi(x, y) = (x + y - 2)^q \Longrightarrow M_{\varphi}(G) = Z_q(G)$.

  (iii) $\varphi(x, y) = xy \Longrightarrow M_{\varphi}(G) = M_2(G)$.

Background and Definitions

- Among these distance-based graph invariants of a graph G, the **Wiener index** $W(G)$, **hyper-Wiener index** $WW(G)$ and **Harary index** $H(G)$ are three famous topological indices, where

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} dist(u,v), \quad H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{dist(u,v)}, \quad \text{and}$$

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{2}\left(dist(u,v) + \left(dist(u,v)\right)^2\right).$$

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$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{2} \left(dist(u,v) + (dist(u,v))^2 \right).$$

- When $\psi(x)$ is a function defined on positive real number x, then the Q-**index** [F.M. Brückler, T. Došlić, A. Graovac, I. Gutman, *Chem. Phys. Lett.*, 2011] $W_\psi(G)$ of G, is constructed as

$$W_\psi(G) = \sum_{\{u,v\} \subseteq V(G)} \psi(dist(u,v)).$$

Background and Definitions

- Let $A(G)$ and $D(G)$ be the adjacent matrix and diagonal matrix of degrees of G, respectively. Then, $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix of G. Denote by $\Theta(G, b)$ be the **largest eigenvalue** of $bD(G) + A(G)$.

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- Let $\rho(G)$ and $\mu(G)$ be the largest eigenvalue of $A(G)$ and $Q(G)$, respectively.

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- Let $\rho(G)$ and $\mu(G)$ be the largest eigenvalue of $A(G)$ and $Q(G)$, respectively.

- It is an interesting problem for us to find a unified method to determine the corresponding extremal graph(s) for as many topological indices and graph spectra as possible in a given graph category.

Definition:

Let $(x) = (x_1, x_2, ..., x_n)$ and $(y) = (y_1, y_2, ..., y_n)$ be two different non-increasing real numbers, we write $(x) \lhd (y)$ if and only if $(x) \neq (y)$, $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, ..., n$. The ordering $\pi \lhd \pi'$ is always called **majorization**.

Majorization theorem

Definition:

Let $\Phi(G)$ be an invariant defined on G. If $\Phi(G)$ is maximum (resp., minimum) among all graphs in a given graph category $\mathcal{G}$, then we call G as a **maximum** (resp., **minimum**) **extremal graph (of $\mathcal{G}$)**.

Definition:

When G and G' are two maximum (resp., minimum) extremal graphs of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, if $\pi \triangleleft \pi'$ implies that relationship $\Phi(G) < \Phi(G')$ (resp., $\Phi(G) > \Phi(G')$), then we say that $\Phi(G)$ **satisfying the majorization theorem**.

Problem:

(i) Which graphical invariants satisfy the majorization theorem?

(ii) In a given graph category, which degree sequence is largest in $\triangleleft$.

Theorem A:

Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. If G and G' are two graphs with $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, then

(i) [M. Liu, B. Liu, *Australas. J. Combin.*, 2010.] $R_q(G) < R_q(G')$ holds for $q < 0$ or $q > 1$, and $R_q(G) > R_q(G')$ holds for $0 < q < 1$.

(ii) $\prod^{q}(G) < \prod^{q}(G')$ holds for $q < 0$, and $\prod^{q}(G) > \prod^{q}(G')$ holds for $q > 0$.

(iii) $\prod_{2}(G) < \prod_{2}(G')$.

(iv) If $f(x)$ is a strictly convex function, then $H_f(G) < H_f(G')$;

(v) If $f(x)$ is a strictly concave function, then $H_f(G) > H_f(G')$.

Theorem B:

Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. Let G and G' be a maximum extremal c-cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively.

(i) [M. Liu, K. Xu, X.-D. Zhang, *DAM*, 2019.] If $\varphi(x, y)$ is a good escalating function, then $M_{\varphi}(G) < M_{\varphi}(G')$ holds for $c \in \{0, 1, 2\}$;

(ii) [M. Liu, B. Liu, *Extremal theory of graph spectrum*, 2018.] If $b \geq 0$ is a real number, then $\Theta(G, b) < \Theta(G', b)$ holds for $c \in \{0, 1\}$;

(iii) [Y. Huang, B. Liu, Y. Liu, *DM*, 2011], [X. Jiang, Y. Liu, B. Liu, *LMA*, 2011] If $c = 2$, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$;

(iv) [X.-M. Zhang, X.-D. Zhang, D. Gray, H. Wang, *J. Graph Theory*, 2013]. If $\psi(x)$ is a nonnegative and nonincreasing function and $c = 0$, then $W_{\psi}(G) < W_{\psi}(G')$ for strictly decreasing function $\psi(x)$.

Majorization Theorems

Theorem C:

Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. Let G and G' be a minimum extremal c-cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively.

(i) [X.-M. Zhang, X.-D. Zhang, D. Gray, H. Wang, *J. Graph Theory*, 2013]. If $\psi(x)$ is a nonnegative and nondecreasing function and $c = 0$, then $W_\psi(G) > W_\psi(G')$ for strictly increasing function $\psi(x)$.

(ii) [M. Liu, F. Li, K.C. Das, *MATCH Commun. Math. Comput. Chem.*, 2013]. If $c \in \{0, 1, 2\}$, then $\overline{M_2(G)} > \overline{M_2(G')}$;

(iii) [M. Liu, F. Li, K.C. Das, *MATCH Commun. Math. Comput. Chem.*, 2013]. If $c \geq 0$, then $\overline{M_1(G)} > \overline{M_1(G')}$.

Majorization Theorems

Definition:

For graph category $\mathcal{G}$, we call G a good extremal graph of $\mathcal{G}$ if G satisfies:
(1) $\Theta(G, b)$ is **largest** in $\mathcal{G}$ for $b \geq 0$ when G is either a tree or a unicyclic graph;
(2) $\rho(G)$ is **largest** in $\mathcal{G}$ when G is a bicyclic graph;
(3) $\mu(G)$ is **largest** in $\mathcal{G}$ when G is a bicyclic graph;
(4) $M_\varphi(G)$ is maximum in $\mathcal{G}$ when $\varphi(x, y)$ is a good escalating function;
(5) $W_\psi(G)$ is maximum in $\mathcal{G}$ when $\psi(x)$ is a strictly decreasing function;
(6) $W_\psi(G)$ is minimum in $\mathcal{G}$ when $\psi(x)$ is a strictly increasing function;
(7) $H_f(G)$ is maximum in $\mathcal{G}$ when $f(x)$ is a strictly convex function;
(8) $H_f(G)$ is minimum in $\mathcal{G}$ when $f(x)$ is a strictly concave function;
(9) $\overline{M_1(G)}$ and $\overline{M_2(G)}$ are minimum in $\mathcal{G}$.

Remark:

Actually, in this paper, we have determined the largest degree sequence in majorization relationship $\triangleleft$ for the c-cyclic graphs with n vertices and given maximum degree, independence number, matching number, number of pendent vertices and given domination number, respectively, where $c \in \{0, 1, 2\}$.

Main results

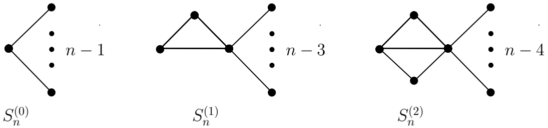

Figure 1: The extremal graphs of trees, unicyclic graphs, bicyclic graphs with n vertices.

Theorem:

If $n \geq 4$ and $c \in \{0, 1, 2\}$, then $S_n^{(c)}$ is the unique good extremal c-cyclic graph among all c-cyclic graphs with n vertices.

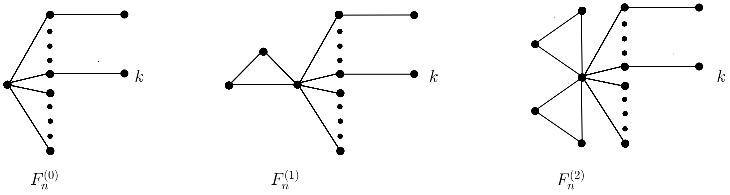

Figure 2: The extremal graphs of trees, unicyclic graphs, bicyclic graphs with k pendant vertices.

Theorem:

If $k \geq 1$ and $c \in \{0,1,2\}$, then $F_n^{(c)}(k)$ is a good extremal c-cyclic graph among all c-cyclic graphs with n vertices and k pendent vertices when $n \geq k+1+2c$.

Remark: Idea comes from [X.-D. Zhang, *Discrete Math.*, 2008], $c=0$; [X.-D. Zhang, *Discrete Appl. Math.*, 2009], $c=1$; [Y. Huang, B. Liu, Y. Liu, *Discrete Math.*, 2011], $c=2$

- Let $V_\Delta(G)$ be the vertex set of G, whose degree is equal to the maximum degree Δ of G. Let $G_M(n,\Delta)$ be the graph satisfies the following four conditions:
  (i) $G_M(n,\Delta)$ is a BFS-graph with the maximum degree vertex v_1 as its root. If $G_M(n,\Delta)$ is a unicyclic graph, then $\mathcal{R}(G_M(n,\Delta)) = C_3$, where $V(C_3) = \{v_1, v_2, v_3\}$; If $G_M(n,\Delta)$ is a bicyclic graph, then $\mathcal{R}(G_M(n,\Delta)) = K_4 - e$;
  (ii) All the pendent vertices of $G_M(n,\Delta)$ lie on the last or the second last layer;
  (iii) If $V\left(\mathcal{R}(G_M(n,\Delta))\right) \not\subseteq V_\Delta(G)$, then all the vertices of $G_M(n,\Delta)$ outside $\mathcal{R}(G_M(n,\Delta))$ are pendent vertices. Furthermore, if $v_2 \notin V_\Delta(G)$, then $d_{G_M(n,\Delta)}(v_3) = 2$ and $G\left[\{v_1, v_2, v_3\}\right] \cong C_3$;

Main results

- If $v_2 \in V_\Delta(G)$, $v_3 \notin V_\Delta(G)$ and $G_M(n,\Delta)$ is a bicyclic graph, then $d_{G_M(n,\Delta)}(v_4) = 2$;

  (iv) All the vertices of $V(G) \setminus \big(V\big(\mathcal{R}(G_M(n,\Delta))\big) \cup V_\Delta(G)\big)$, except for at most one d-vertex, are pendent vertices. Furthermore, if such a d-vertex exists, then it must belong to the second last layer, where $1 < d < \Delta$.

Theorem:

If $\Delta \geq 3$ and $c \in \{0,1,2\}$, then $G_M(n,\Delta)$ is a good extremal graph in the class of c-cyclic graphs with n vertices and maximum degree Δ.

Remark: Idea comes from [X.-D. Zhang, *Discrete Math.*, 2008]. [X.-D. Zhang, *Discrete Appl. Math.*, 2009]. [Y. Huang, B. Liu, Y. Liu, *Discrete Math.*, 2011]

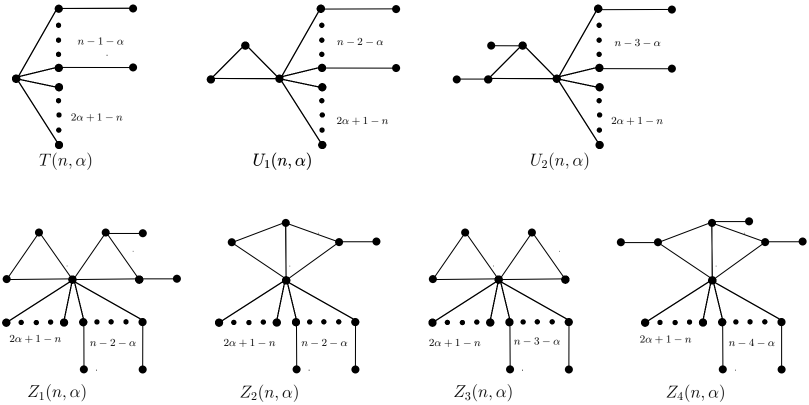

Figure 3: The extremal graphs of trees, unicyclic graphs, bicyclic graphs with independent number α.

Theorem.

The graph G is a good extremal graph in the class of c-cyclic graphs with n vertices and independence number α, where

(i) $G = T(n,\alpha)$ when $c = 0$ and $n \geq 3$;

(ii) $G \in \{U_1(n,\alpha),\ U_2(n,\alpha)\}$ when $c = 1$ and $3 \leq \alpha \leq n-3$;

(iii) $G \in \{Z_1(n,\alpha),\ Z_2(n,\alpha),\ Z_3(n,\alpha),\ Z_4(n,\alpha)\}$ when $c = 2$ and $4 \leq \alpha \leq n-4$.

Remark. Idea comes from [Y. Yao, M. Liu, K.C. Das, Y. Ye, *MATCH Commun. Math. Comput. Chem.*, 2019.]

The main results

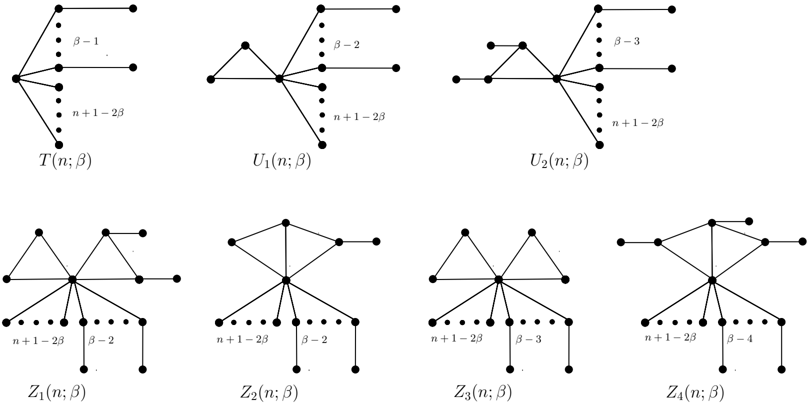

Figure 4: The extremal graphs of trees, unicyclic graphs, bicyclic graphs with matching number β.

The main results

Theorem.

The graph G is a good extremal graph in the class of c-cyclic graphs with n vertices and matching number β, where

(*i*) $G = T(n; \beta)$ when $c = 0$ and $n \geq 3$;

(*ii*) $G \in \{U_1(n; \beta), U_2(n; \beta)\}$ when $c = 1$ and $3 \leq \beta \leq n - 3$;

(*iii*) $G \in \{Z_1(n; \beta), Z_2(n; \beta), Z_3(n; \beta), Z_4(n; \beta)\}$ when $c = 2$ and $4 \leq \beta \leq n - 4$.

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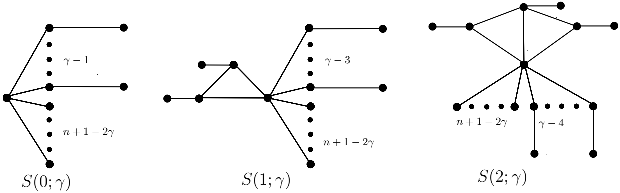

Figure 5: The extremal graphs of trees, unicyclic graphs, bicyclic graphs with dominating number γ.

Theorem.

If $n \geq 3 + 3c$ and $c \in \{0, 1, 2\}$, then $S(c; \gamma)$ is a good extremal graph in the class of c-cyclic graphs with n vertices and dominating number γ.

Some problems under consideration

Problem

Determine the good extremal graph in the class of c-cyclic graphs with given diameter and girth, respectively, for $c \in \{0, 1, 2\}$.

Problem

Determine the extremal graph of $H_f(G)$ in the class of c-cyclic graphs with given different graphical invariants (for instance, the fixed maximum degree, independence number, matching number, domination number, cut-vertices, number of cut edges, number of pendent vertices)

Thank You!