The minimum and maximum graphical function-index spanning tree problems

Yanni Dong[1,2]

[1]Northwestern Polytechnical University
[2]University of Twente

Joint work with Yuhang Bai[1], Hajo Broersma[2] and Shenggui Zhang[1]

May 12, 2022

1. Preliminaries

2. Results

Chemical graph theory

Mathematics subject classification

- **05** (1940-now) **Combinatorics**
  - **05C** (1973-now) **Graph theory**
    - **05C09** (2020-now) **Graphical indices** (Wiener index, Zagreb index, Randić index, etc.)
    - **05C92** (2020-now) **Chemical graph theory**

Some notations

Let $G = (V, E)$ be a graph.

- $d_G(u)$: **the degree of vertex u in G**
- $d_G(u, v)$: **the distance between vertices u and v**
- $\delta_G(u)$: **the distance sum of vertex u in G (i.e, $\delta_G(u) = \sum_{v \in V(G)} d_G(u, v)$)**
- $\mu(G)$: **the cyclomatic number of G (i.e., $\mu(G) = |E(G)| - |V(G)| + 1$)**
- $\lambda_1, \lambda_2, \ldots, \lambda_{|V(G)|}$: **the eigenvalues of adjacency matrix of G**
- $m(G, k)$: **the number of k-matchings of G**
- $i(G, k)$: **the number of k-element independent sets of G**

'

Table 1: Some chemical indices

Name	Expression
Augmented Zagreb index	$AZI(G)=\sum_{u,v\in E(G)}(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2})^3$
Atom-bond connectivity index	$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$
Balaban index	$J(G)=\frac{\lvert E(G)\rvert}{\mu(G)+1}\sum_{uv\in E}\frac{1}{\sqrt{\delta_G(u)\delta_G(v)}}$
Energy	$E(G)=\sum_{i=1}^{n}\lvert\lambda_i\rvert$
Estrada index	$EE(G)=\sum_{i=1}^{n}e^{\lambda_i}$
First Zagreb index	$M_1(G)=\sum_{v\in V(G)}d_G(v)^2$
General first Zagreb index	$M_1^{\alpha}(G)=\sum_{v\in V(G)}d_G(v)^{\alpha}$
General Randić index	$R_{\alpha}(G)=\sum_{uv\in E(G)}(d_G(u)d_G(v))^{\alpha}$
Hosoya index	$Z(G)=\sum_{k\geq 0}m(G,k)$
Hyper-Wiener index	$WW(G)=\sum\limits_{\{u,v\}\subseteq V(G)}d_G(u,v)+\sum\limits_{\{u,v\}\subseteq V(G)}d_G^2(u,v)$
Merrifield-Simmons index	$\sigma(G)=\sum_{k\geq 0}i(G,k)$
Platt index	$P(G)=\sum_{uv\in E(G)}(d_G(u)+d_G(v)-2)$
Randić index	$R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)d_G(v)}}$
Second Zagreb index	$M_2(G)=\sum_{uv\in E(G)}d_G(u)d_G(v)$
Wiener index	$W(G)=\sum_{\{u,v\}\subseteq V(G)}d_G(u,v)$

Categories of indices

These indices can be classified into some categories:

- **degree-based indices;**
- **distance-based indices;**
- **subgraph counting-based indices;**
- **eigenvalue-based indices;**
- **......**

Categories of indices

These indices can be classified into some categories:

- **degree-based indices**;
- distance-based indices;
- subgraph counting-based indices;
- eigenvalue-based indices;
- ......

Graphical function-indices

- Let $f(x)$ be a real function. The graphical function-index $H_f(G)$ of the graph G with vertex-weight function $f(x)$ is defined as

$$H_f(G) = \sum_{u \in V} f(d_G(u)).$$

- Let $f(x, y)$ be a symmetric real function. The graphical function-index $TI_f(G)$ of the graph G with edge-weight function $f(x, y)$ is defined as

$$TI_f(G) = \sum_{uv \in E} f(d_G(u), d_G(v)).$$

- It follows from $\sum_{uv \in E}(\frac{f(d_G(u))}{d_G(u)} + \frac{f(d_G(v))}{d_G(v)}) = \sum_{w \in V} f(d_G(w))$ that $H_f(G)$ is a special case of $TI_f(G)$ (i.e., $f(x, y) = \frac{f(x)}{x} + \frac{f(y)}{y}$).

I. Gutman, Degree-based topological indices, *Croat. Chem. Acta*, 86 (2013) 351–361.

Graphical function-indices

- Let $f(x)$ be a real function. The graphical function-index $H_f(G)$ of the graph G with vertex-weight function $f(x)$ is defined as

$$H_f(G) = \sum_{u \in V} f(d_G(u)).$$

- Let $f(x, y)$ be a symmetric real function. The graphical function-index $TI_f(G)$ of the graph G with edge-weight function $f(x, y)$ is defined as

$$TI_f(G) = \sum_{uv \in E} f(d_G(u), d_G(v)).$$

- It follows from $\sum_{uv \in E}(\frac{f(d_G(u))}{d_G(u)} + \frac{f(d_G(v))}{d_G(v)}) = \sum_{w \in V} f(d_G(w))$ that $H_f(G)$ is a special case of $TI_f(G)$ (i.e., $f(x, y) = \frac{f(x)}{x} + \frac{f(y)}{y}$).

I. Gutman, Degree-based topological indices, *Croat. Chem. Acta*, 86 (2013) 351–361.

Table 2: Some edge-weight functions and related chemical indices

Name	$f(x,y)$
Albertson index	$\|x-y\|$
Arithmetic-geometric index	$(x+y)/2\sqrt{xy}$
Argumented Zagreb index	$x^3y^3/(x+y-2)^3$
Atom-bond connectivity index	$\sqrt{(x+y-2)/(xy)}$
Extended index	$(x/y+y/x)/2$
First Gourava index	$x+y+xy$
First hyper-Gourava index	$(x+y+xy)^2$
First hyper-Zagreb index	$(x+y)^2$
First Zagreb index	$x+y$
Forgotten index	x^2+y^2
Geometric-arithmetic index	$2\sqrt{xy}/(x+y)$
Harmonic index	$2/(x+y)$

Table 2: Some edge-weight functions and related chemical indices

Name	$f(x,y)$
Inverse degree	$x^{-2}+y^{-2}$
Inverse sum index	$xy/(x+y)$
Modified first Zagreb index	$x^{-3}+y^{-3}$
Product-connectivity Gourava index	$\sqrt{(x+y)xy}$
Randić index	$1/\sqrt{xy}$
Reciprocal Randić index	$\sqrt{xy}$
Reciprocal sum-connectivity index	$\sqrt{x+y}$
Second Gourava index	$(x+y)xy$
Second hyper-Gourava index	$x^2y^2(x+y)^2$
Second hyper-Zagreb index	$(xy)^2$
Second Zagreb index	xy
Sigma index	$(x-y)^2$
Sombor index	$\sqrt{x^2+y^2}$
Sum-connectivity index	$1/\sqrt{x+y}$
Sum-connectivity Gourava index	$1/\sqrt{x+y+xy}$

MinGfst and MaxGfst problems

The **minimum** (resp., **maximum**) **graphical function-index spanning tree problem**, **MinGfst** (resp., **MaxGfst**) for short, asks to find a spanning tree whose graphical function-index is as **small** (resp., **large**) as possible.

The decision problem of the **MinGfst** (resp., **MaxGfst**) on **vertex-weight functions**, **D-MinGfst-V** (resp., **D-MaxGfst-V**) for short, is defined as follows.

D-MinGfst-V
INSTANCE: A graph G, and a real number K.
QUESTION: Does G possess a spanning tree T such that $H_f(T) \leq K$?

D-MaxGfst-V
INSTANCE: A graph G, and a real number K.
QUESTION: Does G possess a spanning tree T such that $H_f(T) \geq K$?

The decision problem of the **MinGfst** (resp., **MaxGfst**), **D-MinGfst** (resp., **D-MaxGfst**) for short, is defined similarly as above.

D-3-MinGfst-V problem

- **A graph G is called cubic if $d_G(v) = 3$ for every $v \in V(G)$.**

The decision problem of MinGfst on vertex-weight function for cubic graphs, D-3-MinGfst-V for short, is defined as follows.

> **D-3-MinGfst-V**
> **INSTANCE: A cubic graph G, and a real number K.**
> **QUESTION: Does G possess a spanning tree T such that $H_f(T) \leq K$?**

Results

Theorem 1

If f is a strictly concave (resp., convex) function, then the D-3-MinGfst-V (resp., D-3-MaxGfst-V) problem is $\mathcal{NP}$-complete.

Corollary 1

If f is a strictly concave (resp., convex) function, then the D-MinGfst-V (resp., D-MaxGfst-V) problem is $\mathcal{NP}$-complete.

Spanning tree with no vertices of degree 2 for cubic graphs

The decision problem of spanning tree with no vertices of degree 2 for cubic graphs, D-3-Stwnvd2 for short, known to be $\mathcal{NP}$-complete, is defined as follows.

> **D-3-Stwnvd2**
> **INSTANCE: A cubic graph G.**
> **QUESTION: Does G possess a spanning tree with no vertices of degree 2?**

P. Lemke, ***The Maximum-Leaf Spanning Tree Problem in Cubic Graphs is NP-complete*****, IMA Preprinter Series #428, University of Minnesota, Minneapolis, 1988.**

Results

- P_n: the path on n vertices

Theorem 2

The D-MaxGfst (resp., D-MinGfst) problem is $\mathcal{NP}$-complete if P_n is the unique extremal tree that maximizes (resp., minimizes) its corresponding graphical function-index among trees on n vertices.

Corollary 2

If f is a strictly concave (resp., convex) function, then the D-MaxGfst-V (resp., D-MinGfst-V) problem is $\mathcal{NP}$-complete.

Some indices with the path as the extremal tree

Theorem 3

Among trees on n vertices, P_n is the unique extremal tree with the minimum Balaban index, the maximum energy, the minimum Estrada index, the minimum general first Zagreb index $M_1^{\alpha}(G)$ for $\alpha < 0$ or $\alpha > 1$, the maximum general first Zagreb index $M_1^{\alpha}(G)$ for $0 < \alpha < 1$, the minimum general Randić index $R_{\alpha}(G)$ for $\alpha > 0$ and $n \geq 5$, the maximum general Randić $R_{\alpha}(G)$ for $-\frac{1}{2} \leq \alpha < 0$, the maximum Hosoya index, the maximum hyper-Wiener index, the minimum Merrifield-Simmons index, the minimum second Zagreb index, the maximum Wiener index.

References

K. Das and S.-G. Lee, On the Estrada index conjecture, *Linear Algebra Appl.*, 431 (2009) 1351–1359.

H. Deng, On the Balaban index of trees, *MATCH Commun. Math. Comput. Chem.*, 66 (2011) 253–260.

H. Dong and X. Guo, Character of graphs with extremal Balaban index, *MATCH Commun. Math. Comput. Chem.*, 66 (2010) 799–812.

R.C. Entringer, D.E. Jackson and D.A. Synder, Distance in graphs, *Czech. Math. J.*, 26 (1976) 283–296.

I. Gutman, W. Linert, I. Lukovits, and A.A. Dobrynin, Trees with extremal hyper-Wiener index: mathematical basis and chemical applications, *J. Chem. Inf. Comput. Sci.*, 37 (1997) 349–354.

References

- Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić index, *MATCH Commun. Math. Comput. Chem.*, 52 (2004) 129–146.
- Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić index, *MATCH Commun. Math. Comput. Chem.*, 52 (2004) 119–128.
- R. Lang, X. Li and S. Zhang, Inverse problem for the Zagreb index of molecular graphs, *Appl. Math. J. Chinese Univ. Ser. A*, 18 (2003) 487–493.
- X. Li, Y Shi and I. Gutman, *Graph energy*, Springer, New York, 2012.
- X. Li and J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.*, 50 (2005) 195–208.
- S. Wagner and I. Gutman, Maxima and minima of the Hosoya index and the Merrifield-Simmons index: a survey of results and techniques, *Acta Appl. Math.*, 112 (2010) 323–346.

Hamilton path problem

The decision problem of the **Hamilton path** problem (**D-Hp**), known to be $\mathcal{NP}$**-complete**, is defined as follows.

D-Hp
INSTANCE: A graph G.
QUESTION: Does G have a Hamilton path?

M.R. Garey and D.S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness, A Series of Books in the Mathematical Sciences*, W.H. Freeman and Company, San Francisco, 1979.

Thank you for your attention!