

Relations Between the Product- and Sum-connectivity Indices

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Abstract. Several relations between the product- and sum-connectivity indices are established. (doi: 10.5562/cca2052)

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INTRODUCTION

Let G be a simple graph with vertex-set $V(G)$ and edge-set $E(G)$.¹ For $v \in V(G)$, $\Gamma(v)$ denotes the set of its (first) neighbors in G and the degree of v is $d_v = |\Gamma(v)|$. The product-connectivity index or the Randić connectivity index $R = R(G)$ of G is defined as²

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The product-connectivity index is used successfully in QSPR and QSAR modeling^{3–10} and its mathematical properties have also been studied extensively, as summarized in two monographs.^{11,12}

The sum-connectivity index $\chi = \chi(G)$ of G is defined as¹³

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

The use of sum-connectivity index in QSPR and QSAR modeling has been investigated.^{14–16} As already pointed by Balaban *et al.*,¹⁷ the sum-connectivity index may be considered as a proper topological index¹ (molecular descriptor^{6,7}). Mathematical properties of the sum-connectivity index have also been established.^{18–21} Related to the sum-connectivity index, sum-connectivity matrix and sum-connectivity energy have been proposed.²²

In this note, we establish several relations between the product- and the sum-connectivity indices.

RELATIONS BETWEEN THE PRODUCT- AND SUM-CONNECTIVITY INDICES

Let G be a graph. If G has no pendant vertices (vertices of degree one), then $\chi(G) \geq R(G)$ with equality if and only if all non-isolated vertices have degree two.¹³ Obviously, $d_u + d_v \leq 2d_u d_v$ with equality if and only if $d_u = d_v = 1$. Thus

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \geq \sum_{uv \in E(G)} \frac{1}{\sqrt{2d_u d_v}} = \frac{1}{\sqrt{2}} R(G)$$

with equality if and only if all non-isolated vertices have degree one. If $d_u \geq d_v \geq 1$ and $d_u \geq 2$, then $d_u + d_v \leq \frac{3}{2}d_u d_v$ with equality if and only if $d_u = 2$ and $d_v = 1$. Thus, if G has no components on two vertices, then

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \geq \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{3}{2}d_u d_v}} = \sqrt{\frac{2}{3}} R(G)$$

with equality if and only if all non-trivial components of G are paths on three vertices. Thus we have

Proposition 1. Let G be a graph. Then $\chi(G) \geq \frac{1}{\sqrt{2}} R(G)$ with equality if and only if all non-isolated vertices have degree one. Moreover, if G has no components on two vertices, then $\chi(G) \geq \sqrt{\frac{2}{3}} R(G)$ with equality

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if and only if all non-trivial components of G are paths on three vertices, and if no pendant vertices, then $\chi(G) \geq R(G)$ with equality if and only if all non-isolated vertices have degree two.

Let G be a graph with n vertices and m edges. By Caychy-Schwarz inequality,

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \leq \sqrt{m \sum_{uv \in E(G)} \frac{1}{d_u + d_v}}$$

with equality if and only if the sum of degrees of the two end vertices is a constant for all edges. On the other hand, by the arithmetic-geometric mean inequality,

$$\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \leq \sum_{uv \in E(G)} \frac{1}{2\sqrt{d_u d_v}} = \frac{R(G)}{2}$$

with equality if and only if every component is regular. Combining the above two inequalities, we have

Proposition 2. Let G be a graph with m edges. Then

$$\chi(G) \leq \sqrt{\frac{mR(G)}{2}}$$

with equality if and only if G is regular.

From Theorem 1, upper bounds for the product-connectivity index will result in upper bounds for the sum-connectivity index. We give several such examples.

Recall that $R(G) \leq \frac{n}{2}$ with equality if and only if every component is nontrivial and regular.¹¹ Thus we have

*Corollary 3.*²³ Let G be a graph with n vertices and m edges. Then

$$\chi(G) \leq \frac{\sqrt{nm}}{2}$$

with equality if and only if G is regular.

By Corollary 3, among n -vertex graphs the complete graph is the unique graph with maximum sum-connectivity index, equal to $\frac{n\sqrt{n-1}}{2\sqrt{2}}$,¹³ and among n -vertex bipartite graphs the complete bipartite graph with one partite set with $\lfloor \frac{n}{2} \rfloor$ vertices is the unique graph with maximum sum-connectivity index, equal to $\sqrt{\frac{n}{4} \left\lfloor \frac{n^2}{4} \right\rfloor}$.

Let \bar{G} be the complement of the graph G . Let $\bar{m} = |E(\bar{G})|$. From Corollary 3, we have

$$\begin{aligned} \chi(G) + \chi(\bar{G}) &\leq \frac{\sqrt{n}}{2} (\sqrt{m} + \sqrt{\bar{m}}) \\ &\leq \frac{\sqrt{n}}{2} \cdot \sqrt{2(m + \bar{m})} \\ &= \frac{\sqrt{n}}{2} \cdot \sqrt{n(n-1)} \\ &= \frac{n\sqrt{n-1}}{2} \end{aligned}$$

with equalities if and only if G and \bar{G} are regular and $m = \bar{m}$, i.e., G is regular and $2m = \frac{n(n-1)}{2}$, i.e., G is regular of degree $\frac{n-1}{2}$. Thus we have

Corollary 4. Let G be a graph with n vertices. Then

$$\chi(G) + \chi(\bar{G}) \leq \frac{n\sqrt{n-1}}{2}$$

with equality if and only if G is regular of degree $\frac{n-1}{2}$.

Let G be a graph with n vertices. Recall that $\chi(G) + \chi(\bar{G}) \geq \frac{n\sqrt{n-1}}{2\sqrt{2}}$ with equality if and only if G or \bar{G} is the complete graph.¹³

Let G be a graph with no isolated vertices and clique number ω . A particular result in Reference 24 says $R \leq \frac{\omega-1}{2\omega} \left(\sum_{u \in V(G)} \frac{1}{\sqrt{d_u}} \right)^2$ with equality if and only if G is regular complete ω -partite graph. Thus we have

Corollary 5. Let G be a graph with no isolated vertices, m edges and clique number ω . Then

$$\chi(G) \leq \frac{1}{2} \sqrt{\frac{\omega-1}{\omega}} m \sum_{u \in V(G)} \frac{1}{\sqrt{d_u}}$$

with equality if and only if G is regular complete ω -partite graph.

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REFERENCES

1. N. Trinajstić, *Chemical Graph Theory*, 2nd revised ed., CRC Press, Boca Raton, FL, 1992.
2. M. Randić, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
3. L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.
4. L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure-Activity Analysis*, Research Studies Press/Wiley, Letchworth/New York, 1986.
5. J. Devillers and A. T. Balaban (eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, 1999.
6. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
7. M. V. Diudea (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, Nova, Hungtin, N.Y., 2001.
8. L. Pogliani, *Chem. Rev.* **100** (2000) 3827–3858.
9. M. Randić, *J. Mol. Graph. Model.* **20** (2001) 19–35.
10. R. García-Domenech, J. Gálvez, J. V. de Julián-Ortiz, and L. Pogliani, *Chem. Rev.* **108** (2008) 1127–1169.
11. X. Li and I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, University of Kragujevac, Kragujevac, 2006.
12. I. Gutman and B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, University of Kragujevac, Kragujevac, 2008.
13. B. Zhou and N. Trinajstić, *J. Math. Chem.* **46** (2009) 1252–1270.
14. B. Lučić, N. Trinajstić, and B. Zhou, *Chem. Phys. Lett.* **475** (2009) 146–148.
15. B. Lučić, S. Nikolić, N. Trinajstić, B. Zhou, and S. Ivaniš Turk, in: I. Gutman, and B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications I*, University of Kragujevac, Kragujevac, 2010, pp. 101–136.
16. D. Vukičević and N. Trinajstić, *Croat. Chem. Acta* **83** (2010) 349–351.
17. A. T. Balaban, P. V. Khadikar, and S. Aziz, *Iranian J. Math. Chem.* **1** (2010) 43–67.
18. Z. Du, B. Zhou, and N. Trinajstić, *J. Math. Chem.* **47** (2010) 842–855.
19. R. Xing, B. Zhou, and N. Trinajstić, *J. Math. Chem.* **48** (2010) 583–591.
20. S. Wang, B. Zhou, N. Trinajstić, *Filomat* **25** (no. 3) (2011) 29–42.
21. Z. Du and B. Zhou, *Bull. Malays. Math. Sci. Soc.* **35** (2012) 101–117.
22. B. Zhou and N. Trinajstić, *Acta Chim. Slov.* **57** (2010) 513–517.
23. B. Horoldagva and I. Gutman, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 723–730.
24. B. Zhou and D. Vukičević, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 189–196.