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Edge–decomposition of topological indices

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ABSTRACT The topological indices, defined as the sum of contributions of all pairs of vertices (among which are the Wiener, Harary, hyper–Wiener indices, degree distance, and many others), are expressed in terms of contributions of edges and pairs of edges.

KEYWORDS topological index • molecular graph • edge–decomposition • coindex

1. INTRODUCTION

The structure of organic molecules is often represented by graphs, so-called "molecular graphs" [1]. A graph invariant is a function defined on the graph, that is independent of the labeling of the vertices. In the case of molecular graphs, such invariants are constructed so as to reflect relevant structural features of the underlying chemical species. These graph-based molecular structure descriptors are usually referred to as *topological indices*. More than a thousand topological indices has been proposed until now [2], several of which were found to be successful in chemical, physico–chemical, or pharmacologic applications, especially in QSAR/QSPR studies [3].

Let G be a molecular graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The edge of G, connecting the vertices x and y will be denoted by xy. The degree (= number of first neighbors) of a vertex $x \in V(G)$ will be denoted by $d(x)$.

Many (but not all!) topological indices have one of the following three algebraic forms:

$$TI_1 = TI_1(G) = \sum_{v \in V(G)} F_1(v) \tag{1}$$

$$TI_2 = TI_2(G) = \sum_{uv \in E(G)} F_2(u,v) \tag{2}$$

$$TI_3 = TI_3(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} F_3(u,v) \tag{3}$$

where F_1, F_2, and F_3 are functions dependent of a vertex or on a pair of vertices of the molecular graph G.

For example, $F_1(v)$ is equal to $\varepsilon(v)d(v)$ and $d(v)^3$ in the case of eccentric connectivity index [4] and forgotten index [5], respectively, where $\varepsilon(v)$ stands for the eccentricity of the vertex v. $F_2(u,v)$ is equal to $\frac{1}{\sqrt{d(u)d(v)}}$ and $\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$ in the case of Randić index [6] and augmented Zagreb index [7], respectively. $F_3(u,v)$ is equal to $\delta(u,v), \frac{1}{\delta(u,v)}, \binom{\delta(u,v)}{2}$, and $[d(u)+d(v)]\delta(u,v)$ in the case of Wiener index [8], Harary index [9], hyper–Wiener index [10], and degree distance [11], respectively, where $\delta(u,v)$ stands for the distance between the vertices u and v. There exist, of course, many more TI_3-type topological indices [2].

The vertices and edges of the molecular graph represent the atoms and chemical bonds of the underlying molecule [1]. Bearing this in mind, the term $F_1(v)$ in Eq. (1) may be viewed as the contribution of the respective atom to the topological index TI_1. Analogously, $F_2(u,v)$ is the contribution of the respective chemical bond to TI_2, whereas $F_3(u,v)$ is the contribution of a pair of atoms to the topological index TI_3.

In a recent paper [12], Došlić et al. established a general identity for topological indices of the type TI_1, which we state as follows:

Theorem 1. *Let G be any connected graph, and any of its invariants satisfying Eq. (1). Then*

$$TI_1(G) = \sum_{uv \in E(G)} \left[\frac{F_1(u)}{d(u)} + \frac{F_1(v)}{d(v)} \right]. \tag{4}$$

Formula (4) can be interpreted as the edge-decomposition of a topological index of the type TI_1.In other words, the term $\frac{F_1(u)}{d(u)} + \frac{F_1(v)}{d(v)}$ is the contribution of the chemical bond represented by the edge uv to TI_1.

In what follows we offer an analogous identity for the edge–decomposition of topological indices of the type TI_3.

2. Edge–Based Increments for TI$_3$–type Topological Indices

In Eq. (3), for obvious chemical reasons, it has to be assumed that $F_3(u,v) = F_3(v,u)$. In most of the currently studied topological indices, $F_3(u,u) = 0$ for all vertices u, but we shall consider the general case when $F_3(u,u)$ may be different from zero. Eq. (3) can thus be rewritten as

$$TI_3 = \frac{1}{2} \left[\sum_{u \in V} \sum_{v \in V} F_3(u,v) - \sum_{u \in V} F_2(u,u) \right]. \tag{5}$$

Let $e = uu''$ and $f = vv'$ be two edges of the molecular graph G. Then in view of identity (4), the first term on the right-hand side of (5) is transformed as follows:

$$\begin{aligned}
\sum_{u \in V} \sum_{v \in V} F_3(u,v) &= \sum_{u \in V} \sum_{vv' \in E} \left[\frac{F_3(u,v)}{d(v)} + \frac{F_3(u,v')}{d(v')} \right] = \sum_{vv' \in E} \left[\sum_{u \in V} \frac{F_3(u,v)}{d(v)} + \sum_{u \in V} \frac{F_3(u,v')}{d(v')} \right] \\
&= \sum_{vv' \in E} \sum_{uu' \in E} \left[\frac{F_3(u,v)}{d(u)d(v)} + \frac{F_3(u,v')}{d(u)d(v')} + \frac{F_3(u',v)}{d(u')d(v)} + \frac{F_3(u',v')}{d(u')d(v')} \right] \\
&= \sum_{e \in E} \sum_{f \in E} \gamma(e,f)
\end{aligned}$$

where γ is the term pertaining to the contribution of a pair of edges, defined as

$$\gamma(e,f) = \gamma_G(e,f) = \frac{F_3(u,v)}{d(u)d(v)} + \frac{F_3(u,v')}{d(u)d(v')} + \frac{F_3(u',v)}{d(u')d(v)} + \frac{F_3(u',v')}{d(u')d(v')}. \tag{6}$$

It is easy to verify that $\gamma(e,f) = \gamma(f,e)$. Therefore,

$$\sum_{e\in E}\sum_{f\in E}\gamma(e,f)=2\sum_{\substack{(e,f)\subseteq E\\ e\neq f}}\gamma(e,f)+\sum_{e\in E}\gamma(e,e)\,. \tag{7}$$

Recall that

$$\gamma(e,e)=\frac{F_3(u,u)}{d(u)^2}+\frac{F_3(u',u')}{d(u')^2}+2\frac{F_3(u,u')}{d(u)\,d(u')}\,.$$

Using Eq. (4), the second term on the right–hand side of (5) is directly transformed into

$$\sum_{u\in V}F_3(u,u)=\sum_{uu'\in E(G)}\left[\frac{F_3(u,u)}{d(u)}+\frac{F_3(u',u')}{d(u')}\right] \tag{8}$$

and therefore

$$\sum_{e\in E}\gamma(e,e)=\sum_{u\in V}F_3(u,u)=2\Gamma(e)$$

where Γ is the term pertaining to the contribution of an individual edge, defined as

$$\Gamma(e)=\Gamma_G(e)=\frac{1}{2}\left[\frac{F_3(u,u)}{d(u)^2}+\frac{F_3(u',u')}{d(u')^2}+2\frac{F_3(u,u')}{d(u)\,d(u')}-\frac{F_3(u,u)}{d(u)}-\frac{F_3(u',u')}{d(u')}\right]. \tag{9}$$

Note that for the majority of currently investigated topological indices of the type TI_3 (in particular, for all distance–based indices [13]), $F_3(u,u)=0$ for all vertices $u\in V(G)$. Then the expression (9) for Γ is significantly simplified:

$$\Gamma(e)=\frac{F_3(u,u')}{d(u)\,d(u')}\,.$$

Substituting Eqs. (7) and (8) back into (5), we arrive at our main result.

Theorem 2. *Let G be any connected graph, and* $TI_3(G)$ *any of its invariants satisfying Eq. (3). Then*

$$TI_3(G)=\sum_{e\in E(G)}\Gamma_G(e)+\sum_{\substack{\{e,f\}\subseteq E\\ e\neq f}}\gamma_G(e,f)\,. \tag{10}$$

Theorem 2 can be understood as the extension of Theorem 1 to topological indices of the type TI_3. From formula (10) we see that the edge–dependence of a topological index of the type TI_3 consists of contributions of individual edges, expressed by the terms $\Gamma(e)$, Eq. (9), and of contributions of pairs of edges, expressed by terms $\gamma(e, f)$, Eq. (6).

3. COINDICES

In [14], Došlić put forward the concept of a *topological coindex*. In the case of TI_2–type indices, Eq. (2), the coindex is defined simply as

$$\overline{TI}_2 = \sum_{uv \notin E(G)} F_2(u,v)$$

assuming that $u \neq v$. In the case of a TI_1–type index, the coindex can be conceived by using Theorem 1 as

$$\overline{TI}_1 = \sum_{uv \notin E(G)} \left[\frac{F_1(u)}{d(u)} + \frac{F_1(v)}{d(v)} \right].$$

These coindices, especially in the case of Zagreb indices (when $F_1(u) = d(u)^2$ and $F_2(u,v) = d(u)\,d(v)$), have attracted some attention and have recently been extensively studied, see [15–18] and the references cited therein.

Based on Theorem 2, we can now introduce also the coindices of TI_3–type topological indices:

$$\overline{TI}_3 = \sum_{e \notin E} \Gamma(e) + \sum_{\substack{\{e,f\} \not\subset E \\ e \neq f}} \gamma(e,f)$$

where $\sum_{e \notin E}$ indicates summation of pairs of vertices that are not adjacent in the graph G, and where the meaning of $\sum_{\{e,f\} \not\subset E}$ is analogous.

Finding out whether any of the TI_3–coindices deserves to be further examined remains a task for the future.

REFERENCES

1. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.
2. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

3. J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.
4. V. Sharma, R. Goswami, A. K. Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies, *J. Chem. Inf. Comput. Sci.* **37** (1997) 273–282.
5. B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.
6. M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
7. B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* **48** (2010) 370–380.
8. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
9. D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.
10. D. J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **35** (1995) 50–52.
11. A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.
12. T. Došlić, T. Réti, D. Vukičević, On the vertex degree indices of connected graphs, *Chem. Phys. Lett.* **512** (2011) 283–286.
13. K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, *MATCH Commun. Math. Comput. Chem*. **71** (2014) 461–508.
14. T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.
15. S. M. Hosamani, I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, *Appl. Math. Comput*. **247** (2014) 1156–1160.
16. Ž. Kovijanić Vukićević, G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iranian J. Math. Chem*. **5** (2014) 19–29.
17. I. Gutman, B. Furtula, Ž. Kovijanić Vukićević, G. Popivoda, On Zagreb indices and coindices, *MATCH Commun. Math. Comput. Chem*. **74** (2015) 5–16.
18. A. Maden, E. Kaya, Bounds for the co–PI index of a graph, *Iranian J. Math. Chem*. **6** (2015) 1–13.