ОРИГИНАЛНИ НАУЧНИ РАДОВИ
ОРИГИНАЛЬНЫЕ НАУЧНЫЕ СТАТЬИ
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On vertex and edge degree-based topological indices

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Abstract:

Introduction/purpose: The entire topological indices (TI_{ent}) are a class of graph invariants depending on the degrees of vertices and edges. Some general properties of these invariants are established.

Methods: Combinatorial graph theory is applied.

Results: A new general expression for TI_{ent} is obtained. For triangle-free and quadrangle-free graphs, this expression can be significantly simplified.

Conclusion: The paper contributes to the theory of vertex and edge degree-based graph invariants.

Key words: entire topological index, vertex and edge degree-based graph invariant, degree (of vertex), degree (of edge).

Introduction

In this paper, we are concerned with connected simple graphs. Let G be such a graph, and let $\mathbf{V} = \mathbf{V}(G)$ and $\mathbf{E} = \mathbf{E}(G)$ be its vertex and edge sets, respectively. The graph G has $|\mathbf{V}(G)| = n$ vertices and $|\mathbf{E}(G)| = m$ edges. Two vertices u, v of the graph are said to be adjacent, denoted as $u \sim v$, if u and v are the endpoints of an edge. The respective edge will then be denoted by uv. A vertex u and an edge e are said to be incident, denoted as $u \sim e$, if u is an endpoint of the edge e. Two edges e, f are said to be incident, denoted as $e \sim f$, if the edges e and f have a common vertex as the endpoint.

The degree of a vertex $u \in \mathbf{V}(G)$, denoted as d_u, is the number of vertices of G that are adjacent to u. The degree of an edge $e \in \mathbf{V}(G)$, denoted by d_e, is the number of edges of G that are incident to e. If the endpoints of the edge e are the vertices u and v, then it is easy to see that $d_e = d_u + d_v - 2$.

A graph is said to be regular of degree r if $d_u = r$ holds for all $u \in \mathbf{V}(G)$. A regular graph of degree r with n vertices, has $m = \frac{1}{2}nr$ edges.

The distance between two vertices $u, v \in \mathbf{V}(G)$ (= length of the shortest path connecting u and v) is denoted by $d(u,v)$. If u and v are adjacent, then $d(u,v) = 1$.

For additional details of graph theory, see (Harary, 1969; Bondy & Murty, 1976).

In contemporary graph theory, especially in network theory and chemical graph theory, a large number of invariants of the form

$$TI = TI(G) = \sum_{\substack{x,y \in \mathbf{V}(G) \\ x \sim y}} F(d_x, d_y) \qquad (1)$$

are being considered. They are usually referred to as "'vertex-degree-based topological indices". In formula (1), the summation goes over all pairs of adjacent vertices of the underlying graph G, i.e., over the pairs of vertices at the unit distance, $d(x,y) = 1$. F stands for a real-valued function with the property $F(x,y) = F(y,x)$ and $F(x,y) \geq 0$ for all values of the variables x and y that the vertex degrees of the graph G may assume. Some best known and most studied invariants of this kind are the first Zagreb index ($F = x+y$), the second Zagreb index ($F = xy$), the Randić index ($F = 1/\sqrt{xy}$), the forgotten index ($F = x^2+y^2$), the atom-bond-connectivity index ($F = \sqrt{(x+y-2)/(xy)}$), and the Sombor index ($F = \sqrt{x^2+y^2}$). For details see (Todeschini & Consonni, 2000; Gutman, 2023).

Motivated by the success of both the mathematical theory and (mainly chemical) applications of the vertex-degree-based indices of type (1), their modified version

$$TI_{ve} = TI_{ve}(G) = \sum_{\substack{x \in \mathbf{V}(G)\,,\, e \in \mathbf{E}(G) \\ x \sim e}} F(d_x, d_e) \qquad (2)$$

was put forward, first for $F = x + y$ and $F = xy$ (Kulli, 2016), and recently also for $F = \sqrt{x^2+y^2}$ (Kulli, 2022; Kulli & Gutman, 2022). The latter graph invariant is now called the KG-Sombor index, and is denoted by $KG = KG(G)$ (Kulli & Gutman, 2022; Kulli et al., 2022; Kosari et al., 2023; Madhumitha et al., 2024). In the case of the KG-Sombor index, it has been shown (Kulli et al., 2022; Kulli & Gutman, 2022) that

$$KG(G) = \sum_{\substack{x,y \in \mathbf{V}(G) \\ x \sim y}} \left[\sqrt{d_x^2 + (d_x + d_y - 2)^2} + \sqrt{d_y^2 + (d_x + d_y - 2)^2} \right].$$

It is straightforward to state the generalization of the above formula:

Theorem 1. *Let G be a simple graph. Then the invariant TI_{ve}, Eq. (2), can be expressed solely in terms of the vertex degrees of G, and satisfies the relation*

$$TI_{ve}(G) = \sum_{\substack{x,y \in \mathbf{V}(G) \\ x \sim y}} \Big[F(d_x, d_x + d_y - 2) + F(d_y, d_x + d_y - 2) \Big]. \tag{3}$$

Proof. The edge e in formula (2) has two endpoints, say x and y. Bearing this in mind, the summation in (2), for any particular edge e, must go over both x and y. This results in the two terms on the right-hand side of (3). Formula (3) follows now by taking into account that $d_e = d_x + d_y - 2$ for any edge $e = xy$. □

Entire topological indices

Short time after the vertex– and edge-degree-based graph invariants of the type (2) were conceived (Kulli, 2016), the "entire" topological indices were put forward (Alwardi et al., 2018), first for the choices $F = x + y$ (first Zagreb index) and $F = xy$ (second Zagreb index). Eventually, entire indices were considered for the forgotten index ($F = x^2 + y^2$), (Bharali et al., 2020), the Randić index ($F = 1/\sqrt{xy}$), (Saleh & Cangul, 2021), and quite recently for the Sombor index ($F = \sqrt{x^2 + y^2}$), (Movahedi & Akhbari, 2023).

The general form of these indices is

$$TI_{ent} = TI_{ent}(G) = \sum_{\substack{x,y \in \mathbf{V}(G) \cup \mathbf{E}(G) \\ x \sim y}} F(d_x, d_y). \tag{4}$$

Before stating Theorem 2, we recall some basic facts on line graphs (Harary, 1969; Bondy & Murty, 1976).

The line graph $L(G)$ of the graph G is defined so that its vertex set is $\mathbf{E}(G)$, and two vertices of $L(G)$ are adjacent if the respective edges of G are incident. Thus the line graph of the graph G has $|\mathbf{E}(G)| = m$ vertices and $m(L(G)) = \sum_{u\in\mathbf{V}(G)} \binom{d_u}{2}$ edges.

Theorem 2. *Let G be a simple graph and let $L(G)$ be its line graph. Then the invariant TI_{ent}, Eq. (4), can be expressed solely in terms of the vertex degrees of G and $L(G)$, and satisfies the relation*

$$TI_{ent} = TI_{ent}(G) = \sum_{\substack{x,y\in\mathbf{V}(G)\\ x\sim y}} \Big[F(d_x, d_y) + F(d_x, d_x + d_y - 2) + F(d_y, d_x + d_y - 2)\Big] + \sum_{\substack{x,y\in\mathbf{V}(L(G))\\ x\sim y}} F(d_x, d_y)\,. \quad (5)$$

Proof. It is evident that the summation on the right-hand side of (4) can be divided into three parts, namely for

(a) $x \in \mathbf{V}(G)$ and $y \in \mathbf{V}(G)$
(b) $x \in \mathbf{V}(G)$ and $y \in \mathbf{E}(G)$ or vice versa;
(c) $x \in \mathbf{E}(G)$ and $y \in \mathbf{E}(G)$

In view of Eq. (1), the component of TI_{ent} pertaining to (a) is equal to TI, i.e.,

$$\sum_{\substack{x,y\in\mathbf{V}(G)\\ x\sim y}} F(d_x, d_y) \quad (6)$$

whereas by Eqs. (2) and (3), the component pertaining to (b) is equal to TI_{ve}, i.e.,

$$\sum_{\substack{x,y\in\mathbf{V}(G)\\ x\sim y}} \Big[F(d_x, d_x + d_y - 2) + F(d_y, d_x + d_y - 2)\Big]\,. \quad (7)$$

The component of TI_{ent}, corresponding to the choice of pairs of incident edges, namely (c), is equal to the TI-index of the line graph of the graph G:

$$\sum_{\substack{x,y\in\mathbf{V}(L(G))\\ x\sim y}} F(d_x, d_y) \quad (8)$$

Combining (6)–(8), we arrive at

$$TI_{ent}(G) = TI(G) + TI_{ve}(G) + TI(L(G))$$

from which Eq. (5) directly follows. □

Special cases of expressions (6) and (8) were recognized by the authors of the earlier papers on entire topological indices (Alwardi et al., 2018; Bharali et al., 2020; Saleh & Cangul, 2021; Movahedi & Akhbari, 2023), but no one of them was aware of formula (7).

Theorem 2, and in particular formula (7), are stated here for the first time.

Corollary 1. *If G is a regular graph of the degree r, with n vertices and m edges, then*

$$TI_{ent}(G) = \frac{1}{2}nr\big[F(r,r) + 2F(r,2r-2) + (r-1)\,F(2r-2,2r-2)\big]\,.$$

Proof. In formula (5), all vertex degrees of G are equal to r, whereas all vertex degrees of $L(G)$ are equal to $2r-2$. The first summation in (5) goes over $m = \frac{1}{2}nr$ terms, whereas the second summation goes over $m(L(G)) = \frac{1}{2}nr(r-1)$ terms. □

In the case of triangle-free and quadrangle-free graphs (such are the trees, hexagonal systems, fullerene graphs, nanotubes, etc.), formula (5) can be simplified. Namely, the entire topological indices TI_{ent} of triangle-free and quadrangle-free graphs can be expressed in terms of vertex degrees of the underlying graph G, without any reference to its line graph $L(G)$.

Corollary 2. *If G is a triangle-free and quadrangle-free graph, then Eq. (9) holds:*

$$\begin{aligned} TI_{ent} = TI_{ent}(G) \;&=\; \sum_{\substack{x,y\in\mathbf{V}(G)\\ x\sim y}} \Big[F(d_x,d_y) + F(d_x,d_x+d_y-2) + \\ &+\; F(d_y,d_x+d_y-2)\Big] + \\ &+\; \sum_{\substack{u,v\in\mathbf{V}((G))\\ d(u,v)=2}} F(d_u+d_w-2,d_v+d_w-2) \qquad (9)\end{aligned}$$

where w is the (unique) vertex lying between the vertices u and v.

Proof. If the graph G does not contain triangles and quadrangles, then two vertices at distance 2, say u and v, have a unique vertex between them, say w. Then uw and vw form a pair of incident edges, resulting in

$$\sum_{\substack{x,y \in \mathbf{V}(L(G)) \\ x \sim y}} F(d_x, d_y) = \sum_{\substack{u,v \in \mathbf{V}((G)) \\ d(u,v)=2}} F(d_u + d_w - 2, d_v + d_w - 2)\,. \tag{10}$$

Substituting (10) back into (5) yields (9). □

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О топологических индексах, зависящих от степеней вершин и ребер

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РУБРИКА ГРНТИ: 27.29.19 Краевые задачи и задачи на собственные значения для обыкновенных дифференциальных уравнений и систем уравнений

ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Все топологические индексы (TI_{ent}) *представляют собой класс инвариантов графа, зависящих от степеней расположения вершин и ребер. Установлены некоторые общие свойства этих инвариантов.*

Методы: В данной статье применяется комбинаторная теория графов.

Результаты: Получено новое обобщенное выражение для TI_{ent}. *Для графов без треугольников и четырехугольников это выражение может быть значительно упрощено.*

Выводы: Данная статья вносит вклад в теорию инвариантов графов, зависящих от степеней вершин и ребер.

Ключевые слова: полный топологический индекс, инварианты графов, зависящих от степеней вершин и ребер, степень (вершины), степень (ребра).

О тополошким индексима који зависе од степена чворова и грана

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ОБЛАСТ: математика
КАТЕГОРИЈА (ТИП) ЧЛАНКА: оригинални научни рад

Сажетак:

Увод/циљ: Потпуни тополошки индекси (TI_{ent}) *образују класу графовских инваријанти који зависе од степена чворова и степена грана. Установљене су неке опште особине ових инваријанти.*

Методе: Примењивани су поступци комбинаторне теорије графова.

Резултати: Нађена је нова општа формула за TI_{ent}. *За графове без троуглова и четвороуглова ова формула се значајно поједностављује.*

Закључак: Рад доприноси теорији графовских инваријанти који зависе од степена чворова и степена грана.

Кључне речи: потпуни тополошки индекси, графовске инваријанте које зависе од степена чворова и грана, степен (чвора), степен (гране).

EDITORIAL NOTE: The author of this article, Ivan Gutman, is a current member of the Editorial Board of the Military Technical Courier. Therefore, the Editorial Team has ensured that the double blind reviewing process was even more transparent and more rigorous. The Team made additional effort to maintain the integrity of the review and to minimize any bias by having another associate editor handle the review procedure independently of the editor – author in a completely transparent process. The Editorial Team has taken special care that the referee did not recognize the author's identity, thus avoiding the conflict of interest.

КОММЕНТАРИЙ РЕДКОЛЛЕГИИ: Автор данной статьи Иван Гутман является действующим членом редколлегии журнала «Военно-технический вестник». Поэтому редколлегия провела более открытое и более строгое двойное слепое рецензирование. Редколлегия приложила дополнительные усилия для того чтобы сохранить целостность рецензирования и свести к минимуму предвзятость, вследствие чего второй редактор-сотрудник управлял процессом рецензирования независимо от редактора-автора, таким образом процесс рецензирования был абсолютно прозрачным. Редколлегия во избежание конфликта интересов позаботилась о том, чтобы рецензент не узнал кто является автором статьи.

РЕДАКЦИЈСКИ КОМЕНТАР: Аутор овог чланка Иван Гутман је актуелни члан Уређивачког одбора Војнотехничког гласника. Због тога је уредништво спровело транспарентнији и ригорознији двоструко слепи процес рецензије. Уложило је додатни напор да одржи интегритет рецензије и необјективност сведе на најмању могућу меру тако што је други уредник сарадник водио процедуру рецензије независно од уредника аутора, при чему је тај процес био апсолутно транспарентан. Уредништво је посебно водило рачуна да рецензент не препозна ко је написао рад и да не дође до конфликта интереса.

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