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# Degree-based topological indices: Optimal trees with given number of pendents

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ABSTRACT

A dynamic programming method is elaborated, enabling the characterization of trees with a given number of pendent vertices, for which a vertex-degree-based invariant ("topological index") achieves its extremal value. The method is applied to the chemically interesting and earlier much studied such invariants: the first and second Zagreb index, and the atom–bond connectivity index.



## 1. Introduction

During recent decades, topological indices are being widely used in studies of quantitative structure–property relation (QSPR) and quantitative structure–activity relations (QSAR) [1–5]. Numeric characteristics of graphs representing chemical compounds appear to be good descriptors of various physical, chemical, and biological properties of diverse classes of organic and inorganic substances. Nowadays, hundreds of topological indices have been developed [3,4], from the simplest indices like the count of atoms in a molecule, to pretty complicated ones, e.g. those based on spectral properties of chemical graphs and indices accounting for the heterogeneity of atoms and bonds in a molecule.

QSPR is recognized to be a promising strategy for rational design of materials. In many cases, design of a material with prescribed requirements, can be formulated as an optimization problem – finding, within some class of chemical substances, the species which maximizes or minimizes a certain topological index (or a composition of indices) and satisfying constraints on some other topological indices or their compositions.

The present paper extends a toolkit of topological indices optimization by developing minimization routines for an important class of the, so called, degree-based topological indices [6,7], over the set of acyclic graphs with the fixed number of pendent vertices. In addition, we study index optimization over the set of chemical trees (i.e., trees with the vertex degree limited by 4).

In Section 2 we propose a simple routine characterizing the set of trees that minimize a general first–Zagreb–like index over the set of trees with fixed number of pendent vertices. Then we show how this routine works for the first Zagreb index $M_1$ and for the multiplicative second Zagreb index.

In Section 3 we employ dynamic programming to characterize the set of second Zagreb index ($M_2$) minimizers over the set of all trees with a fixed number of pendent vertices. We also determine the set of atom–bond connectivity (*ABC*) index minimizers over the set of chemical trees with a fixed number of pendent vertices. The same line of reasoning can, in

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principle, be applied to any second–Zagreb–like index. In Section 4 we discuss the limitations of such an approach, using the *ABC* index as an example.

## 2. First–Zagreb–like indices

Let $G$ be a simple connected undirected graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $d_G(v)$ the degree of a vertex $v \in V(G)$ in the graph $G$, i.e., the number of vertices being adjacent to $v$. The vertex $v \in V(G)$ is said to be *pendent* if $d_G(v) = 1$. All other vertices of the graph $G$ are referred to as *non-pendent*. By $W(G)$ we denote the set of all pendent vertices of a graph $G$, and by $M(G) = V(G) \setminus W(G)$ the set of all its non-pendent vertices.

**Definition 1.** The generalized first Zagreb index is

$$C_1(G) := \sum_{v \in V(G)} c(d_G(v))$$

where $c(d)$ is a non-negative function defined for $d \in \mathbb{N}$, and $c(2) > 0$.

Recall that the choice $c(d) = d^2$ yields the "classical" first Zagreb index $M_1$, whose theory is nowadays well elaborated; see the surveys [7–9] and the recent papers [10–12]. The choices $c(d) = \ln d$ and $c(d) = d \ln d$ give the logarithms of the Narumi–Katayama and second multiplicative Zagreb indices; for details see [13,14] and [15,16], respectively.

A tree is a connected graph with $N$ vertices and $N - 1$ edges. Let $\mathcal{T}(n)$ be the set of all trees with $n \geqslant 2$ pendent vertices, and define $\mathcal{T}^*(n) := \mathrm{Argmin}_{T \in \mathcal{T}(n)} C_1(T)$, the set of all $C_1$-minimizers in $\mathcal{T}(n)$. In what follows we characterize $\mathcal{T}^*(n)$.

A tree in which all non-pendent vertices have degree $d$ will be called a $d$-tree.

**Lemma 1.** *If $T \in \mathcal{T}^*(n)$, then $d_T(v) \neq 2$ for all $v \in V(G)$.*

**Proof.** Assume the opposite, i.e., that $d_T(v) = 2$. Thus, $v$ would have exactly two neighbors (say, $u_1$ and $u_2$) in $T$. Construct a tree $T'$ by deleting the vertex $v$ and its incident edges and by adding an edge $u_1u_2$ instead. We see that $T' \in \mathcal{T}(n)$, as $T'$ is a tree with exactly $n$ pendent vertices. Since $c(2) > 0$, $C_1(T') = C_1(T) - c(2) < C_1(T)$, and $T$ cannot be optimal. This contradiction completes the proof. □

It is known that for an arbitrary tree $T \in \mathcal{T}(n)$

$$\sum_{m \in M(T)} [d_T(m) - 2] = n - 2 \tag{1}$$

and, vice versa, for each integer $q \geqslant 1$ and a sequence $d_1, \ldots, d_q$, $d_i \geqslant 2$, $i = 1, \ldots, q$, such that $\sum_{i=1}^{q}(d_i - 2) = n - 2$, there exists a tree with $n$ pendent vertices and $q$ non-pendent vertices of degrees $d_1, \ldots, d_q$.

**Lemma 2.** *If $T \in \mathcal{T}^*(n)$, then $|M(T)| \leqslant n - 2$, with equality if $T$ is a 3-tree.*

**Proof.** From Lemma 1, $d_T(m) - 2 \geqslant 1$ for all $m \in M(T)$, and, thus, the left side of (1) is not less than $|M(T)|$. Therefore, $|M(T)| \leqslant n - 2$, and the equality holds when $d_T(m) - 2 = 1$ for all $m \in M(T)$, i.e., if $T$ is a 3-tree. □

For any $n \geqslant 3$, there exists at least one 3-tree.

Consider the following integer program:

$$C_1^* = n\,c(1) + \min_{q=1,\ldots,n-2} \min_{d_1,\ldots,d_q} \left\{ \sum_{i=1}^{q} c(d_i) : d_i \in \mathbb{N},\ d_i \geqslant 3,\ \sum_{i=1}^{q} d_i = 2q + n - 2 \right\}. \tag{2}$$

Let $\mathcal{P}(n)$ be the set of vectors $(q, d_1, \ldots, d_q)$ delivering the minimum in (2). For $n \geqslant 3$ and each tree $T \in \mathcal{T}^*(n)$ with $q$ non-pendent vertices of degrees $d_1, \ldots, d_q$, the vector $(q, d_1, \ldots, d_q)$ belongs to $\mathcal{P}(n)$. Vice versa, each $(q, d_1, \ldots, d_q) \in \mathcal{P}(n)$ gives rise to the set of all trees $\mathcal{T}(n)$ with $q$ non-pendent vertices having degree sequence $d_1, \ldots, d_q$. All these trees minimize $C_1(\cdot)$ and, thus, belong to $\mathcal{T}(n)$. So, the problem of enumerating trees from $\mathcal{T}(n)$ is reduced to characterizing the vectors from $\mathcal{P}(n)$.

Below we first find all optimal vertex degrees $d_1, \ldots, d_q$, provided the number of vertices $q$ is given (see Lemma 3 below). Then we find the optimal number of vertices $q$ (see Theorem 1 below).

Define

$$C_1^*(q) = n\,c(1) + \min_{d_1,\ldots,d_q} \left\{ \sum_{i=1}^{q} c(d_i) : d_i \in \mathbb{N},\ d_i \geqslant 3,\ \sum_{i=1}^{q} d_i = 2q + n - 2 \right\}. \tag{3}$$

This expression gives a part of integer program (2): $C_1^* = \min_{q=1,\ldots,n-2} C_1^*(q)$.