Lanzhou index

Vukičević, Damir; Li, Qiuli; Sedlar, Jelena; Došlić, Tomislav

MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **80** (2018) 863-876

ISSN 0340 - 6253

Lanzhou Index

Damir Vukičević[1], Qiuli Li[2], Jelena Sedlar[3], Tomislav Došlić[4]

[1]*Department of Mathematics, University of Split, R. Boškovića 33, 21000 Split, Croatia*

[2]*School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P. R. China*

[c]*Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Matice hrvatske 15, 21000 Split, Croatia*

[4]*Department of Mathematics, Faculty of Civil Engineering, University of Zagreb, Kačićeva 26, 10000 Zagreb, Croatia*

(Received April 7, 2017)

Abstract

We introduce and investigate a new topological index, the Lanzhou index, and show that it outperforms several existing indices on some benchmark datasets recommended by the *International Academy of Mathematical Chemistry*. We determine its extremal values and characterize extremal graphs, trees, and restricted trees.

Nothing speaks more on the quality of proposed analytic potentials for water than the fact that there are more than seven hundreds of them in the literature.

Anonymous

1 Introduction

A spectre is haunting Mathematical Chemistry – the spectre of proliferation of Topological Indices[1]. Like the water potentials (see [4] for situation some 15 years ago), hundreds and

[1]Paraphrased after the first sentence of *The Communist Manifesto* by K. Marx and F. Engels.

thousands of them are clogging the literature, and new ones keep appearing with every new issue of several research journals. Even some of their most ardent one-time proponents and promoters now recognize that something must be done in order to keep the field from descending into chaos. Milan Randić, for example, compiled a list of commandments (twelve of them) that a new quantity must fulfill to be worth of study [11]. Others, like Ivan Gutman, took a more proactive approach, touring mathematical chemistry conferences and advocating restrain in introducing new and investigating existing topological indices [6, 7]. According to Gutman's views, only the quantities that outperform the best of currently known topological indices in modeling some chemically relevant property deserve to be introduced and studied. In addition, he approves of publishing results on already existing indices only if they are deep enough and mathematically interesting. The main purpose of this note is to show that those requirements, strict as they are, are reasonable and not impossible to meet. We introduce a new topological index, show that it behaves better than the existing ones in predicting a chemically relevant property, and we also establish mathematically interesting results concerning the extremal structures.

2 Definitions and preliminary results

We start by introducing some notation. For a given graph G, its vertex set is denoted by $V(G)$ and its edge set by $E(G)$. The **degree** of a vertex $u \in V(G)$ is equal to the number of its neighbors and we denote it by d_u. The complete graph, the path, and the star on n vertices are denoted by K_n, P_n, and S_n, respectively, while T_n denotes a generic tree on n vertices. By $K_{m,n}$ we denote the complete bipartite graph with classes of bipartition of sizes m and n. The **complement graph** $\overline{G}$ of a graph G has the same vertex set $V(G)$, and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G. The **first Zagreb index** $M_1(G)$ of a graph G is defined as

$$M_1(G) = \sum_{u \in V(G)} d_u^2,$$

while the **forgotten index** of G is defined as

$$F(G) = \sum_{u \in V(G)} d_u^3.$$

We notice that $M_1(G)$ and $F(G)$ are defined in a similar way. Indeed, they were defined in the same paper [10], but their fortunes since have been remarkably different. While

the first Zagreb index became one of the most popular and well researched topological indices, the other one fell into oblivion and remained there until very recently, when it was reintroduced by Furtula and Gutman [3].

As mentioned before, Ivan Gutman has been arguing for quite some time that only those new descriptors which outperform the existing ones deserve to be introduced and further studied. As a part of this effort, he and his collaborators recently published several papers trying to identify well performing descriptors among the existing ones and to provide a set of benchmark values of correlation coefficients that any new descriptors should aim to exceed [5, 8, 9]. Most of those papers were concerned with degree-based indices [1, 2] similar to those mentioned above and to the one we will consider later in this paper. A nice example of that approach is the above-mentioned paper on the forgotten index [3], which contains a section dedicated to justification of the new index by demonstrating its chemical usefulness. The predictive ability of the forgotten index was tested by comparing it with the first Zagreb index on the benchmark dataset of 18 octane isomers recommended by the *International Academy of Mathematical Chemistry*. It was found that their predictive powers are quite similar, with both indices performing well (i.e., yielding the correlation coefficient greater than 0.95) on the same two properties and yielding no satisfactory correlation on eleven others. It turned out, however, that for one of the remaining properties, (the logarithm of) the octanol-water partition coefficient P, an excellent correlation was obtained by a linear combination of $M_1(G)$ and $F(G)$ of the form $M_1(G)+\lambda F(G)$, where λ was a free parameter ranging from -20 to 20. A sharp peak was obtained at $\lambda = -0.140$ (see Fig. 2 of [3]), leading to the expression $0.2058(M_1(G) - 0.14F(G)) + 7.5864$ for $\log P$, with the absolute value of the correlation coefficient equal to 0.99896 and the mean absolute percentage error of 0.06%. No explanation was offered for the value of λ resulting in such an excellent agreement with experimental values of $\log P$.

One of our goals here is to eliminate the need of a free parameter λ in $M_1(G) - \lambda F(G)$ by offering an explanation for the observed value of λ in terms intrinsic to graph(s) under consideration. More precisely, we will define a new topological index without free parameters that (almost) outperforms $M_1(G) - 0.14F(G)$ on the same dataset, and that significantly outperforms it on a larger one.

Crucial for our goal is the observation that the optimal value of $\lambda_{opt} = -0.140$ is, by

absolute value, very close to 1/7, the reciprocal value of the largest possible degree of a vertex in a simple graph on 8 vertices. By interpreting λ_{opt} as $-1/(n-1)$ and by multiplying through by $n-1$ to get rid of fractions, we come to consider a quantity defined as

$$(n-1)M_1(G) - F(G) = \sum_{u \in V(G)} d_u^2[(n-1) - d_u] = \sum_{u \in V(G)} \overline{d_u} d_u^2,$$

where by $\overline{d_u}$ we denote the degree of u in $\overline{G}$, the complement of G. We denote the newly defined quantity by $Lz(G)$ and call it the **Lanzhou index** of G. (The name was chosen since the observation was made and subsequent work was done in the city of Lanzhou in China during a visit of Croatian researchers within the scope of a bilateral Croatian-Chinese research project mentioned in the Acknowledgment.) Hence,

$$Lz(G) = \sum_{u \in V(G)} \overline{d_u} d_u^2.$$

3 Main results

3.1 Justification

Our first task is to justify the new index by demonstrating its predictive ability for a chemically relevant property of a non-trivial class of molecules. We have already mentioned that our new index, the Lanzhou index, almost outperforms the Furtula - Gutman linear combination $M_1(G) - 0.14F(G)$. By "almost" we mean that Lanzhou index yields slightly smaller absolute value of the correlation coefficient, namely 0.96693 instead of Furtula - Gutman's 0.99896. We admit that the correlation is a bit weaker for the Lanzhou index. However, we believe that the slightly poorer correlation coefficient is by far outweighed by elimination of the free parameter, and, consequently, by far wider range of applications. To illustrate our point, we have compared performances of the first Zagreb index $M_1(G)$, the forgotten index $F(G)$, the Furtula - Gutman linear combination $M_1(G) - 0.14F(G)$, and the Lanzhou index $Lz(G)$ in predicting the logarithm of the octanol-water partition coefficient for 32 (out of 35) nonane isomers. Additionally, as a kind of control, we have performed the same computations for an ad-hoc quantity $\overline{Lz}(G)$ defined by switching the roles of degrees of vertices in a graph and in its complement, $\overline{Lz}(G) = \sum_{u \in V(G)} d_u \overline{d_u}^2$. The results are summarized in Table 1. (The first four values of the upper row are as reported in [3].)

	M_1	F	$M_1 - 0.140F$	Lz	$\overline{Lz}$
octanes	-0.07933	0.00550	-0.99876	-0.96693	0.16616
nonanes	-0.78729	-0.73379	-0.65970	-0.98869	0.82598

Table 1. Comparison of correlation coefficients of five indices for the octanol-water partition coefficient of octane and nonane isomers.

Several interesting things can be gleaned from Table 1. As expected, neither $M_1(G)$ nor $F(G)$ perform well for nonanes. However, their linear combination with Furtula - Gutman's value of the free parameter performs even worse. This indicates that the octane-optimal value $\lambda_{opt} = -0.140$ is not suitable for other numbers of vertices. On the contrary, when replaced by $-1/8$, yielding thus the Lanzhou index, it yields a very good correlation coefficient. That also indicates that the scaling with the number of vertices is well described by the factor of $-1/(n-1)$. The rightmost column was computed in order to asses the sensitivity of our definition to switching the roles of degrees in a graph and in its complement. The performance of this quantity, a kind of Lanzhou coindex, is consistently (and significantly) worse than for Lanzhou index, indicating thusly that our definition, arbitrary as it seems to be, captures something relevant for determination of the octanol-water partition coefficient.

We have tried to asses the performance of Lanzhou index also for larger molecules. However, our efforts were hampered by lack of reliable data on octanol-water partition coefficients for branched isomers of decanes and larger alkanes. On the lower end (i.e., for heptanes and hexanes) we found that the Lanzhou index performs poorly. We ascribe the poor performance to a very narrow range of values (only two different values for nine heptanes) and small number of isomers.

3.2 Extremal graphs, trees and chemical trees

In this subsection we study some of mathematical properties of Lanzhou index. In particular, we determine its extremal values over general graphs, trees, and trees with maximum degree at most four, and characterize the extremal cases.

We start by stating several results that can be verified by direct computation.

Proposition 1

$Lz(K_n) = Lz(\overline{K_n}) = 0$;

$Lz(K_{m,n}) = mn(2mn - m - n)$;

$Lz(P_n) = 2(n-2)(2n-5)$;

$Lz(S_n) = (n-1)(n-2)$. ■

Next we state the extremal values of Lanzhou index for general graphs and characterize the extremal cases.

Proposition 2

Let G be a graph on n vertices. Then

$$0 \leq Lz(G) \leq \frac{4}{27}n(n-1)^3.$$

The left inequality is satisfied if and only if G is either complete or empty graph. The right inequality is satisfied if and only if $n \equiv 1 \pmod 3$ and G is r-regular with $r = \frac{2}{3}(n-1)$.

Proof

We denote by $c(x) = x^2(n-1-x)$ the contribution of a vertex of degree x to the value of $Lz(G)$. Since $c(x)$ is non-negative for all values of $0 \leq x \leq n-1$, the only way to get zero is to have all vertex contributions equal to zero. Hence, the complete graph and its complement are the only graphs on n vertices whose Lanzhou index is equal to zero.

On the other hand, the largest possible contribution of a vertex to $Lz(G)$ will be for vertices of degree equal to the zero(s) of $c'(x)$. Since $c'(x) = x(2(n-1) - 3x)$, its only non-zero root is integer if and only if $n-1$ is divisible by 3, hence the second claim holds.

■

Nice class of extremal graphs are circulant graphs C^k_{3k+1}, the k-th powers of cycles on $3k+1$ vertices. (The k-th power G^k of G is obtained from G by adding edges between all pairs of vertices at distance at most k in G.)

Now we turn our attention to trees. As all trees on at most 4 vertices belong to the cases covered in Proposition 1, in the rest we consider only trees on $n \geq 5$ vertices.

A **double star** $S_{k,l}$ is a tree obtained from K_2 by attaching $k-1$ leaves to one of its vertices and $l-1$ leaves to the other one. Hence, $S_{k,l}$ has one vertex of degree k, one of degree l, and $k+l-2$ vertices of degree one. A double star on n vertices is **balanced** if the difference between k and l is the smallest possible. Depending on parity of n, this difference will be either zero for an even n or one for an odd n. Hence, a balanced double star on n vertices is either $S_{n/2,n/2}$ or $S_{(n-1)/2,(n+1)/2}$. When the parity of n is not important, we denote the balanced double star on n vertices by $BDS(n)$.

The following result is readily verified by direct computation.

Proposition 3

$$Lz(S_{n/2,n/2}) = \frac{n^3}{4} + \frac{n^2}{2} - 4n + 4;$$
$$Lz(S_{(n-1)/2,(n+1)/2}) = \frac{n^3}{4} + \frac{n^2}{2} - \frac{17}{4}n + \frac{7}{2}.$$

■

We are going to show that the balanced double stars maximize the Lanzhou index over all trees on n vertices for large enough n, while the minimum value is achieved for ordinary stars S_n for all n.

Proposition 4

Let T_n be a tree on $n \geq 15$ vertices. Then

$$Lz(S_n) \leq Lz(T_n) \leq Lz(BDS(n)).$$

The lower bound is achieved if and only if $T_n = S_n$, while the upper bound is achieved if and only if $T_n = BDS(n)$.

Proof

Let $V = V(T_n)$ be the vertex set of T_n. It can be decomposed as $V = L \cup R$, where L is the set of leaves and R the set of non-leaves of T_n. Let $l = |L|$ and $r = |R|$ be the cardinalities of L and R, respectively. Starting from

$$\sum_{u \in R} d_u + l = 2n - 2$$

and rewriting it as

$$\sum_{u \in R} (d_u - 2) + 2(n - l) + l = 2n - 2,$$

we arrive at

$$\sum_{u \in R} (d_u - 2) = l - 2. \tag{1}$$

Now we recall our definition of $c(x)$, the contribution of a vertex of degree x to $Lz(T_n)$. As in the general case, $c(x) = x^2(n - 1 - x)$. In particular, contributions of each of the leaves are given by $c(1) = n - 2$. Now we have

$$Lz(T_n) = \sum_{u \in V} c(d_u) = \sum_{u \in R} c(d_u) + (l - 2)c(1) + 2c(1).$$

By expressing $l - 2$ via (1) we obtain

$$Lz(T_n) = \sum_{u \in R} [c(d_u) + (d_u - 2)c(1)] + 2c(1). \tag{2}$$

We wish to maximize the sum on the right hand side of the above equation. By taking into account

$$\sum_{u\in R}(d_u-2+1)=l-2+r,$$

we arrive at

$$\sum_{u\in R}(d_u-1)=n-2. \tag{3}$$

Now we write $Lz(T_n)$ by taking equation (2) and multiplying each term in the sum by $\frac{d_u-1}{d_u-1}$, thus obtaining

$$Lz(T_n)=\sum_{u\in R}\frac{c(d_u)+(d_u-2)c(1)}{d_u-1}(d_u-1)+2c(1). \tag{4}$$

We define a function $\lambda(x)$ by

$$\lambda(x)=\frac{c(x)+(x-2)c(1)}{x-1}$$

and denote by λ^+ and λ^- its maximum and minimum value, respectively, over all positive integer values of argument yielding non-negative values of $\lambda(x)$. Hence,

$$\lambda^+=\max_{d_u}\lambda(d_u),\qquad \lambda^-=\min_{d_u}\lambda(d_u).$$

Clearly,

$$\lambda^-\sum_{u\in R}(d_u-1)+2c(1)\le Lz(T_n)\le\lambda^+\sum_{u\in R}(d_u-1)+2c(1),$$

and then, by (3),

$$\lambda^-\cdot(n-2)+2c(1)\le Lz(T_n)\le\lambda^+\cdot(n-2)+2c(1).$$

But $\lambda(x)$ is, in fact, a quadratic polynomial with negative leading coefficient, since $x=1$ is a root of its numerator. It can be explicitly written as

$$\lambda(x)=-x^2+(n-2)x+2(n-2).$$

By checking its values at $x=2$ and $x=n-1$ we immediately obtain $\lambda^-=\lambda(n-1)=n-3$. Hence,

$$Lz(T_n)\ge\lambda^-\cdot(n-2)+2c(1)=(n-3)(n-2)+2(n-2)=(n-1)(n-2)=Lz(S_n).$$

So, the Lanzhou index is minimized for stars and only for stars.

Let us now turn our attention to finding the trees maximizing the Lanzhou index. We first suppose that n is even. Then the maximum value of $\lambda(x)$ is achieved for $x = \frac{n-2}{2}$, and values of $\lambda(x)$ are symmetric with respect to $x = \frac{n}{2}-1$. In particular, $\lambda(\frac{n}{2}-1) = \frac{n^2}{4}+n-3$, $\lambda(\frac{n}{2}) = \lambda(\frac{n}{2}-2) = \frac{n^2}{4}+n-4$ and $\lambda(\frac{n}{2}+1) = \lambda(\frac{n}{2}-3) = \frac{n^2}{4}+n-7$. Hence $\lambda^+ = \lambda(\frac{n}{2}-1)$, leading to the upper bound

$$Lz(T_n) \leq \frac{n^3}{4} + \frac{n^2}{2} - 3n + 2.$$

This upper bound is a bit larger than the value achieved by $Lz(S_{n/2,n/2})$; the difference is equal to $n-2$. In order to prove our claim we must show that no other tree has the Lanzhou index closer to the upper bound than the balanced double star.

So, let us suppose that $S_{n/2,n/2}$ is not the extremal tree. Formula (3) implies that any extremal tree T_e can contain at most two vertices of high degree (here by high degree we mean the degree of of $\frac{n}{2}$, $\frac{n}{2}-1$ or $\frac{n}{2}-2$). Since T_e is not equal to $S_{n/2,n/2}$, at least one of those two vertices must have the degree strictly smaller than $\frac{n}{2}$. If none of them has degree equal to $\frac{n}{2}-1$, it follows from relation (4) and Proposition 3 that $Lz(T_e)$ cannot exceed $Lz(S_{n/2,n/2})$. Hence we have three possible cases.

Case 1.

T_e contains a vertex of degree $n/2$. Both that vertex and the vertex of degree $\frac{n}{2}-1$ must be in R. Since the sum of $d_u - 1$ over all vertices in R must be equal to $n-2$, R must contain a vertex of degree 2. All other vertices of T_e must be leaves. Now by direct computation we obtain

$$Lz(T_e) = \frac{n^3}{4} + \frac{n^2}{4} - \frac{n}{2} - 6 < Lz(S_{n/2,n/2})$$

for large enough n (say, $n \geq 11$), a contradiction.

Case 2.

T_e contains two vertices of degree $\frac{n}{2}-1$. Now the sum of their degrees is $n-2$ and R must contain either two additional vertices of degree 2 or one additional vertex of degree 3. In both cases we obtain that the Lanzhou indices of those trees have the same leading cubic term as $Lz(S_{n/2,n/2})$, while no quadratic term is present. Hence in both cases they remain smaller than $Lz(S_{n/2,n/2})$ for large enough n, yielding again a contradiction.

Case 3.

T_e contains a vertex of degree $n/2-1$ and a vertex of degree $n/2-2$. Since the sum of their degrees gives only $n-3$, there must be additional vertices in R. There are three

possible situations: three vertices of degree 2, one vertex of degree 3 and one of degree 2, or just one vertex of degree 4. In all three cases direct computation verifies that their Lanzhou indices do not exceed $Lz(S_{n/2,n/2})$.

Hence the balanced double star $S_{n/2,n/2}$ has the maximum Lanzhou index among all trees on an even number of vertices. The case of an odd number of vertices follows in the same manner and we omit the details. ■

It remains to consider the trees with less than 15 vertices. We say that a tree $T_n \neq BDS(n)$ is **excessive** if $Lz(T_n) > Lz(BDS(n))$. If $Lz(T_n) \geq Lz(BDS(n))$, we say that T_n is **weakly excessive**. It follows from Proposition 4 that the number of excessive and of weakly excessive trees is finite. Furthermore, there are no excessive nor weakly excessive trees on more than 14 vertices. We have computed Lanzhou index for all trees on at most 14 vertices. The results are summarized in Table 2. Its columns give the number of vertices n, the total number of trees $t(n)$, the number of weakly excessive trees $t_{we}(n)$, the number of excessive trees $t_{ex}(n)$, the number of trees maximizing the Lanzhou index $t_{max}(n)$ (excluding the balanced double star), the maximum value of Lanzhou index over all trees on n vertices $Lz_{max}(n)$, and Lanzhou index of the balanced double star $Lz(BDS(n))$.

n	$t(n)$	$t_{we}(n)$	$t_{ex}(n)$	$t_{max}(n)$	$Lz_{max}(n)$	$Lz(BDS(n))$
4	2	0	0	0	12	12
5	3	1	1	1	30	26
6	6	2	2	1	56	52
7	11	7	6	6	90	84
8	23	16	12	1	138	132
9	47	29	24	2	196	188
10	106	21	2	2	270	264
11	235	14	6	1	360	350
12	551	4	4	2	464	460
13	1301	9	2	2	588	582
14	3159	1	0	1	732	732

Table 2. Statistics of weakly excessive, excessive, and extremal trees, and maximum value of Lanzhou index for trees on $4 \leq n \leq 14$ vertices.

Hence, there are altogether 104 weakly excessive and 59 excessive trees. For all $5 \leq n \leq 13$, (and only for those values), the Lanzhou index is maximized by an excessive tree, while for $n = 14$ there is also one weakly excessive tree with maximum value. The unique

maximizing trees for $n = 5$ and 6 are respective paths P_5 and P_6. Other 16 excessive trees maximizing Lanzhou index for a given number of vertices are shown in Fig. 1.

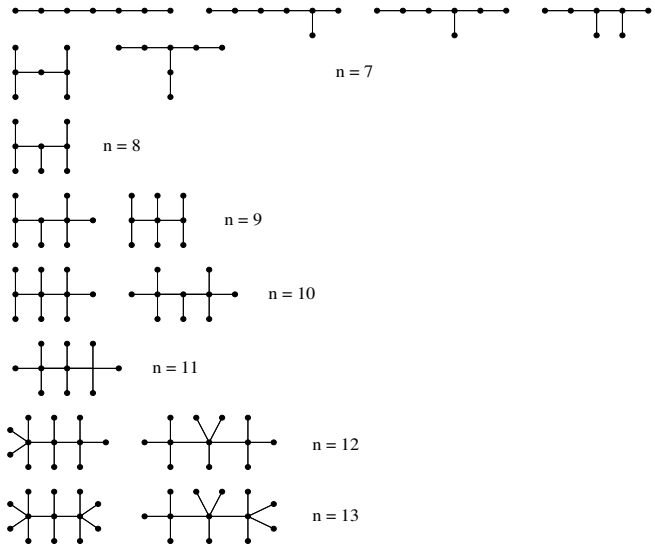

Figure 1. Excessive trees maximizing Lanzhou index.

Similar analysis could be employed to find the extremal graphs and values of Lanzhou index over unicyclic graphs and over other classes of graphs with low connectivity. As an example, we determine extremal values and structures for Lanzhou index over all chemical trees, i.e., the trees whose maximum degree does not exceed four.

Let $\mathcal{T}_n^{\Delta}$ denote the set of all trees on n vertices with maximum degree at most Δ. The smallest interesting case is $\Delta = 3$, while for $\Delta = 4$ we obtain the class of chemical trees. We consider $\Delta = 3$ first.

Let $T_n \in \mathcal{T}_n^3$ and let t denote the number of vertices of degree 3 in T_n. If we denote the number of leaves by l, it follows from

$$3t + 2(n - t - l) + l = 2(n - 1)$$

that $l = t + 2$. The smallest possible value of t is zero, the largest is given by $t = \frac{n-2}{2}$ for even and $t = \frac{n-3}{2}$ for odd values of n. It is easy to see that for any even n there always exist a tree with maximum possible number of vertices of degree 3; it suffices to start from $T_4 = K_{1,3}$, and construct T_{n+2} by adding a pair of leaves to one leaf of T_n. A similar

construction will work for odd n, starting from T_5, the only tree on 5 vertices with one vertex of degree 3.

Proposition 5

Let $n \geq 8$ be an integer and $T_n \in \mathcal{T}_n^3$. Then

$$4n^2 - 18n + 20 \leq Lz(T_n) \leq 5n^2 - 27n + 34 - (n-7)\frac{1-(-1)^n}{2}.$$

The left inequality is satisfied if and only if $T_n = P_n$. The right inequality is satisfied for any tree without vertices of degree 2 if n is even, and for any tree with exactly one vertex of degree 2 if n is odd.

Proof

By direct computation we readily obtain

$$Lz(T_n) = 9t(n-4) + 4(n-2t-2)(n-3) + (t+2)(n-2) = 2(n-7)t + Lz(P_n),$$

and hence

$$Lz(T_n) - Lz(P_n) = 2(n-7)t.$$

The right hand side is an increasing function of t for a fixed $n \geq 8$. It is minimized for the smallest and maximized for the largest possible value of t. That immediately proves the left inequality and yields the equality case. The right inequality now follows by plugging in the largest possible value of t and expressing the results in a more compact form. ■

The case of chemical trees $\mathcal{T}_n^4$ is a bit more complicated, but it follows along the same lines. Let $T_n \in \mathcal{T}_n^4$ and let f and t denote the number of vertices of degree 4 and 3, respectively. Then the number of leaves is given by $l = 2f + t + 2$ and the number of vertices of degree 2 is equal to $n - 3f - 2t - 2$. Again, by direct computation, it follows

$$Lz(T_n) - Lz(P_n) = 6(n-8)f + 2(n-7)t.$$

As both expressions on the right hand side are increasing in f and t for $n \geq 8$, it follows immediately that for large enough n the Lanzhou index of chemical trees on n vertices is minimized by P_n and only by P_n.

In order to find the maximum values and the corresponding structures, one would need to maximize $6(n-8)f + 2(n-7)t$ over all integer f and t satisfying the constraint $3f + 2t \leq n + 2$. However, a quick glance at the linear relaxation of this problem suffices to convince one that it always pays of to maximize f. Indeed, the contribution of a pair

of vertices of degrees 4 and 2 always exceeds the contribution of two vertices of degree 3. Hence, the right hand side will be maximized for all chemical trees containing the maximum possible number of vertices of degree 4. Such trees can be constructed starting from the smallest such trees on 5, 6, and 7 vertices, by adding three leaves on one chosen leaf. The maximum number of vertices of degree 4 in a chemical tree on n vertices is given by $\frac{n-2}{3}$, $\frac{n-3}{3}$ and $\frac{n-4}{3}$ if $n \equiv 2 \pmod 3$, $n \equiv 0 \pmod 3$, and $n \equiv 1 \pmod 3$, respectively. In all cases, the leading term in $Lz(T_n)$ is given by $6n^2$. We omit the lower order terms. We summarize our results for chemical trees.

Proposition 6

Let $n \geq 8$ be an integer and $T_n \in \mathcal{T}_n^4$. Then

$$4n^2 - 18n + 20 \leq Lz(T_n) \leq 6n^2 + O(n).$$

The left inequality is satisfied if and only if $T_n = P_n$. The maximum value of $Lz(T_n)$ is achieved for any tree having the largest possible number of vertices of degree 4 for a given n. ■

For a general Δ, the largest possible number of vertices of degree Δ in a tree on n vertices is of the order of $\frac{n}{\Delta-1}$, and their collective contribution to $Lz(T_n) - Lz(P_n)$ is of the order of $\frac{(\Delta-2)^2+\Delta-2}{\Delta-1}n^2$. That leads to

$$Lz(T_n) - Lz(P_n) = \frac{(\Delta-2)^2 + \Delta - 2}{\Delta - 1}n^2 + O(n)$$

for large enough n, yielding the leading term of $\left(\frac{(\Delta-2)^2+\Delta-2}{\Delta-1} + 4\right) n^2$ for the maximum values of $Lz(T_n)$ over all trees of maximum degree at most Δ.

4 Conclusion

We have introduced and investigated the Lanzhou index, a new topological index that describes a chemically relevant property better than previously available topological indices. In that way we have demonstrated that introducing and studying new topological indices is not incompatible with parsimony principles advocating by Ivan Gutman. The main idea behind our new index is elimination of a free parameter by interpreting it in terms of parameters intrinsic to graphs under consideration. We believe that our approach could be successfully emulated on several classes of so called variable indices which depend on free parameter(s).

Acknowledgment: This work has been supported in part by Croatian Science Foundation under the project 8481 (BioAmpMode). Also, the authors gratefully acknowledge partial support from Croatian-Chinese bilateral project No. 7-22 "Graph-theoretical methods for nanostructures and nanomaterials". This work was also supported by NSFC (Grant no. 11401279) and the Fundamental Research Funds for the Central Universities (Grant no. lzujbky-2016-102)

References

[1] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex-degree-based molecular structure descriptors, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 613–626.

[2] T. Došlić, T. Reti, D. Vukičević, On vertex degree indices of connected graphs, *Chem. Phys. Lett.* **512** (2011) 283–286.

[3] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[4] B. Guillot, A reappraisal of what we have learnt during three decades of computer simulations on water, *J. Mol. Liq.* **101** (2002) 219–260.

[5] B. Furtula, I. Gutman, M. Dehmer, On structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.* **219** (2013) 8973–8978.

[6] I. Gutman, personal communication, Tianjin, 2016.

[7] I. Gutman, personal communication, Leipzig, 2016.

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

[9] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex-degree-based topological indices, *J. Serb. Chem. Soc.* **78** (2013) 805–810.

[10] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[11] M. Randić, Molecular bonding profiles, *J. Math. Chem.* **19** (1996) 375–392.