Weakly Discriminating Vertex–Degree–Based Topological Indices

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Abstract

Let \mathcal{G}_n be the set of graphs with n vertices and $\mathcal{H} \subseteq \mathcal{G}_n$. For each $H \in \mathcal{H}$, let $m(H) = \{m_{i,j}(H)\}$, where $m_{i,j}(H)$ is the number of edges in H that join a vertex of degree i with a vertex of degree j. A vertex-degree-based (VDB, for short) topological index φ is discriminating over \mathcal{H} if non-isomorphic graphs in \mathcal{H} have different values of φ . We say that φ is *weakly discriminating* over \mathcal{H} if the following weaker condition is satisfied for every $H, H' \in \mathcal{H}$:

$$\varphi(H) = \varphi(H') \Longleftrightarrow m(H) = m(H').$$

Let \mathcal{CT}_n be the set of chemical trees with *n* vertices. In this paper we show that many of the well-known VDB topological indices are *not* weakly discriminating over \mathcal{CT}_n . However, the recently introduced Sombor index is weakly discriminating over \mathcal{CT}_n . Also, we give conditions under which a VDB topological index φ is weakly discriminating over an arbitrary class $\mathcal{H} \subseteq \mathcal{G}_n$.

1 Introduction

Throughout this paper a graph G = (V, E) is simple, undirected and unweighted, where V is the set of vertices and E the set of edges. If there is an edge from vertex u to vertex v we indicate this by writing uv (or vu). The degree of the vertex v of G is denoted by d_v . A vertex v is isolated if $d_v = 0$. We denote by $n_i = n_i(G)$ the number of vertices of G with degree i and $m_{i,j} = m_{i,j}(G)$ the number of edges in G joining vertices of degree i and j.

Topological indices are molecular descriptors which play an important role in theoretical chemistry, especially in QSPR/QSAR research [22, 23]. One important class of topological indices are the so-called vertex-degree based (VDB, for short) topological indices (see [10, 18], and for recent results [1, 3, 5–7, 15–17, 24]).

Let \mathcal{G}_n be the set of graphs with *n* non-isolated vertices and $\mathcal{H} \subseteq \mathcal{G}_n$. Let $\Delta = \max \{ \Delta(H) : H \in \mathcal{H} \}$. Consider the set

$$K = \{(i, j) \in \mathbb{N} \times \mathbb{N} : 1 \le i \le j \le \Delta\}$$

lexicographically ordered. Let $h = |K| = \frac{\Delta(\Delta+1)}{2}$. Define the function $m : \mathcal{H} \longrightarrow \mathbb{R}^h$ by $m(H) = (m_{i,j}(H))_{(i,j)\in K}$, where $H \in \mathcal{H}$. Formally, a VDB topological index is a function $T_{\varphi} : \mathcal{H} \longrightarrow \mathbb{R}$ induced by a vector $\varphi \in \mathbb{R}^h$, defined for $H \in \mathcal{H}$ as

$$T_{\varphi}(H) = m\left(H\right) \cdot \varphi, \tag{1}$$

where "." denotes the dot product over \mathbb{R}^h . For brevity, we simply write

$$\varphi(H) = m(H) \cdot \varphi, \tag{2}$$

and say that φ is a VDB topological index defined over \mathcal{H} . Most of the well-known VDB topological indices studied in mathematical chemistry are induced by symmetric functions of the form $\varphi(x, y)$. In other words, the vector $\varphi \in \mathbb{R}^h$ has components $(\varphi(x, y))_{(x,y)\in K}$, where $\varphi(x, y)$ is a symmetric function.

From expression (2), we easily deduce that if $H, H' \in \mathcal{H}$, then [19]

$$\varphi\left(H\right) = \varphi\left(H'\right) \Longleftrightarrow \left[m\left(H\right) - m\left(H'\right)\right] \cdot \varphi = 0 \Longleftrightarrow \left[m\left(H\right) - m\left(H'\right)\right] \perp \varphi.$$

For the well-known VDB topological indices $\varphi \in \mathbb{R}^h$, the perpendicularity condition above occurs very frequently in most of the important classes of sets \mathcal{H} studied (connected graphs, trees, chemical graphs, etc ...). In other words, non-isomorphic graphs of \mathcal{H} have equal value φ . This degeneracy property has been investigated extensively in mathematical chemistry [8,9,13].

In [19], the concept of discrimination of a VDB topological index was generalized to equivalence relations defined in \mathcal{H} . Specifically, if ~ is an equivalence relation defined in \mathcal{H} , then φ discriminates on \mathcal{H} with respect to ~ if the following condition holds: for all $H, H' \in \mathcal{H}$,

$$\varphi\left(H\right) = \varphi\left(H'\right) \Longleftrightarrow H \sim H'$$

In this case we say that φ is discriminating over \mathcal{H} with respect to the equivalence relation \sim . When we consider the isomorphism relation \simeq on \mathcal{H} , then we recover the usual concept of discrimination. But there are other interesting equivalence relations, for example, in [19, Example 2.2] we consider the equivalence relation defined on \mathcal{H} ,

$$H \sim H' \Longleftrightarrow m(H) = m(H'). \tag{3}$$

If a vertex-degree-based topological index φ is discriminating over \mathcal{H} with respect to the relation (3), then we simply say that φ is *weakly discriminating* over \mathcal{H} . Since

$$H \simeq H' \Longrightarrow m(H) = m(H'),$$

it follows that if φ is discriminating over \mathcal{H} (in the usual way), then φ is weakly discriminating over \mathcal{H} .

Naturally a question arises: which VDB topological indices are weakly discriminating over \mathcal{H} ? In Section 2 we study the case $\mathcal{H} = \mathcal{CT}_n$, the set of chemical trees with *n* vertices. Specifically, we show in Examples 2.1 and 2.2 several well-known VDB topological indices which are *not* weakly discriminating over \mathcal{CT}_n : the Randić index [20], the first Zagreb index [12], the sum-connectivity index [25], the harmonic index [26], first hyper-Zagreb index [21], and the reciprocal sum-connectivity index [15]. On the other hand, we show in Theorem 2.3, that the recently introduced Sombor index [11] is weakly discriminating over \mathcal{CT}_n .

In Section 3 we give conditions under which a VDB topological index φ is weakly discriminating over an arbitrary class $\mathcal{H} \subseteq \mathcal{G}_n$. Concretely, we show that if the components $\{\varphi_{i,j}\}_{(i,j)\in K}$ of φ are linearly independent over the set of integers \mathbb{Z} , then φ is weakly discriminating over \mathcal{H} . As a byproduct, we show that if the components $\{\varphi_{i,j}\}_{(i,j)\in K}$ are distinct algebraic numbers, then the exponential e^{φ} is weakly discriminating over \mathcal{H} .

2 Weakly discriminating VDB topological indices over \mathcal{CT}_n

Which VDB topological indices are weakly discriminating over \mathcal{H} ? Let us see some examples when $\mathcal{H} = \mathcal{CT}_n$, the set of chemical trees with *n* vertices. In this case

$$K = \{(i, j) \in \mathbb{N} \times \mathbb{N} : 1 \le i \le j \le 4\}$$

and since $m_{1,1}(T) = 0$ for all $T \in \mathcal{CT}_n$ when $n \ge 3$, all VDB topological indices φ are vectors in \mathbb{R}^9 :

$$\varphi = (\varphi_{1,2}, \varphi_{1,3}, \varphi_{1,4}, \varphi_{2,2}, \varphi_{2,3}, \varphi_{2,4}, \varphi_{3,3}, \varphi_{3,4}, \varphi_{4,4}).$$

Example 2.1 The Randić index is induced by the symmetric function $\varphi(x, y) = \frac{1}{\sqrt{xy}}$, so its associated vector is

$$\varphi = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{8}}, \frac{1}{3}, \frac{1}{\sqrt{12}}, \frac{1}{4}\right).$$

It turns out that the Randić index is not weakly discriminating over CT_n . In fact, consider the trees S and T depicted in Figure 1. Let p be a positive integer. In the tree S there are 4p + 1 vertices of degree 4. In the tree T there are 3p + 1 vertices of degree 4, there is a path with $p \ge 1$ edges between vertices u and v, and there is a path with p edges between vertices w and z. By a counting argument, one easily sees that S and T are trees with 20p + 9 vertices. Moreover,

$$m_{1,2}(S) = 8p + 4, \quad m_{2,4}(S) = 8p + 4, \quad m_{4,4}(S) = 4p,$$

and $m_{i,j}(S) = 0$ for all other values of i, j. On the other hand,

$$m_{1,2}(T) = 6p + 4, \quad m_{2,2}(T) = 2p, \quad m_{2,4}(T) = 12p + 4,$$

and $m_{i,j}(T) = 0$ for all other values of i, j. In particular, $m(S) \neq m(T)$. However,

$$\varphi(S) = \varphi(T) = \left(6\sqrt{2} + 1\right)p + 3\sqrt{2}$$

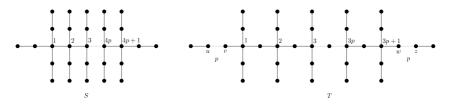


Figure 1. Trees with equal Randić index but different *m*-structure.

Example 2.2 Consider the following VDB topological indices induced by the function $\varphi(x, y)$:

$\varphi\left(x,y ight)$	Name
x + y	first Zagreb index
$(x+y)^2$	first hyper-Zagreb index
$\frac{1}{\sqrt{x+y}}$	sum-connectivity index
$\sqrt{x+y}$	reciprocal sum-connectivity index
$\frac{2}{x+y}$	harmonic index

All these VDB topological indices have the following property in common:

$$\varphi(1,3) = \varphi(2,2); \quad \varphi(1,4) = \varphi(2,3); \quad \varphi(2,4) = \varphi(3,3).$$
 (4)

Hence, for every $U \in \mathcal{CT}_n$,

So a condition that implies that two trees $S, T \in \mathcal{CT}_n$ have equal value of φ is the following:

$$m_{1,3}(S) + m_{2,2}(S) = m_{1,3}(T) + m_{2,2}(T); m_{1,4}(S) + m_{2,3}(S) = m_{1,4}(T) + m_{2,3}(T); m_{2,4}(S) + m_{3,3}(S) = m_{2,4}(T) + m_{3,3}(T); m_{i,j}(S) = m_{i,j}(T) \text{ for the other values of } (i, j) \in K.$$

$$(5)$$

Consider the trees $S, T \in CT_n$ shown in Figure 2. There is a path with $p \ge 1$ edges between vertices u and v in the tree S, and there is a path with p+6 edges between vertices w and z in the tree T. Note that

$$\begin{split} m_{1,2}\left(S\right) &= 2; \quad m_{1,3}\left(S\right) = 6; \quad m_{1,4}\left(S\right) = 0; \quad m_{2,2}\left(S\right) = p; \quad m_{2,3}\left(S\right) = 4; \\ m_{2,4}\left(S\right) &= 0; \quad m_{3,3}\left(S\right) = 4; \quad m_{3,4}\left(S\right) = 0; \quad m_{4,4}\left(S\right) = 0, \end{split}$$

and

$$m_{1,2}(T) = 2;$$
 $m_{1,3}(T) = 0;$ $m_{1,4}(T) = 4;$ $m_{2,2}(T) = p + 6;$ $m_{2,3}(T) = 0;$
 $m_{2,4}(T) = 4;$ $m_{3,3}(T) = 0;$ $m_{3,4}(T) = 0;$ $m_{4,4}(T) = 0.$

Clearly, conditions (5) hold so $\varphi(S) = \varphi(T)$. However, $m(S) \neq m(T)$, which implies that none of these VDB topological indices are weakly discriminating over \mathcal{CT}_n .

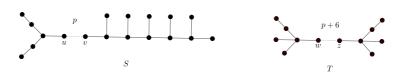


Figure 2. Trees with equal φ but different *m*-structure.

Hence, many of the well known VDB topological indices are *not* weakly discriminating over \mathcal{CT}_n , as we have seen in the previous examples. However, the Sombor index is weakly discriminating over \mathcal{CT}_n , as we shall see in our next result. Recall that the Sombor index is induced by the symmetric function $SO(x, y) = \sqrt{x^2 + y^2}$, so the SO vector is given by

$$SO = \left(\sqrt{5}, \sqrt{10}, \sqrt{17}, 2\sqrt{2}, \sqrt{13}, 2\sqrt{5}, 3\sqrt{2}, 5, 4\sqrt{2}\right).$$
(6)

If T is a chemical tree with n vertices, then

$$SO(T) = \sqrt{5} (m_{1,2} + 2m_{2,4}) + \sqrt{2} (2m_{2,2} + 3m_{3,3} + 4m_{4,4}) + \sqrt{10}m_{1,3} + \sqrt{17}m_{1,4} + \sqrt{13}m_{2,3} + 5m_{3,4}.$$
(7)

We will also use the following well-known relations:

1

$$2m_{1,1} + m_{1,2} + m_{1,3} + m_{1,4} = n_1$$

$$m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2$$

$$m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3$$

$$m_{1,4} + m_{2,4} + m_{3,4} + 2m_{4,4} = 4n_4$$
(8)

Theorem 2.3 The Sombor index SO is weakly discriminating over \mathcal{CT}_n .

Proof. Let $T \in \mathcal{CT}_n$ and set $m_{i,j} = m_{i,j}(T)$ and $n_i = n_i(T)$. By (8),

$$2n = 12 (n_1 + n_2 + n_3 + n_4)$$

= $18p + 6q - 10m_{3,3} - 18m_{4,4} - 27m_{2,4}$
 $+ 16m_{1,3} + 15m_{1,4} + 10m_{2,3} + 7m_{3,4},$ (9)

where

$$p = m_{1,2} + 2m_{2,4} \tag{10}$$

and

$$q = 2m_{2,2} + 3m_{3,3} + 4m_{4,4}.$$
(11)

Assume now that $T' \in \mathcal{CT}_n$ is such that SO(T) = SO(T'). Set $m'_{i,j} = m_{i,j}(T')$ and $n'_i = n_i(T')$. Since

$$\left\{5, \sqrt{2}, \sqrt{5}, \sqrt{10}, \sqrt{13}, \sqrt{17}\right\}$$

is a linearly independent set over \mathbb{Z} , it follows by (7) that

$$p = m'_{1,2} + 2m'_{2,4} \tag{12}$$

$$q = 2m'_{2,2} + 3m'_{3,3} + 4m'_{4,4} \tag{13}$$

and

$$m_{1,3} = m'_{1,3}, \quad m_{1,4} = m'_{1,4} m_{2,3} = m'_{2,3}, \quad m_{3,4} = m'_{3,4}.$$
(14)

Again by (8), (12), (13), and (14),

$$12n = 12 (n'_{1} + n'_{2} + n'_{3} + n'_{4})$$

= $18p + 6q - 10m'_{3,3} - 18m'_{4,4} - 27m'_{2,4}$
 $+16m_{1,3} + 15m_{1,4} + 10m_{2,3} + 7m_{3,4}.$ (15)

Now from relations (9) and (15) we conclude that

$$10\left(m_{3,3} - m_{3,3}'\right) + 18\left(m_{4,4} - m_{4,4}'\right) + 27\left(m_{2,4} - m_{2,4}'\right) = 0.$$
 (16)

The general solution of the Diophantine equation

$$10x + 18y + 27z = 0$$

is

$$\left. \begin{array}{c} x = -54 + 54k \\ y = 27 - 27k \\ z = 2 - 2k \end{array} \right\},$$
(17)

where $k \in \mathbb{Z}$. Hence, from (16) we deduce

$$m_{3,3} - m'_{3,3} = -54 + 54k, \tag{18}$$

$$m_{4,4} - m'_{4,4} = 27 - 27k, \tag{19}$$

$$m_{2,4} - m'_{2,4} = 2 - 2k, (20)$$

for some $k \in \mathbb{Z}$. On the other hand, from (11), (13), and (17),

$$2(m_{22} - m'_{22}) = 3(m'_{3,3} - m_{3,3}) + 4(m'_{4,4} - m_{4,4})$$

= 3(54 - 54k) + 4(-27 + 27k).

Hence,

$$m_{2,2} - m'_{2,2} = 27 - 27k.$$
⁽²¹⁾

Now by (10), (12), and (17),

$$m_{1,2} - m'_{1,2} = 2(m'_{2,4} - m_{2,4}) = 2(2k - 2).$$

Consequently,

$$m_{1,2} - m'_{1,2} = 4k - 4. (22)$$

From (14),

$$m_{1,3} - m'_{1,3} = 0 (23)$$

$$m_{1,4} - m_{1,4}' = 0 (24)$$

$$m_{2,3} - m_{2,3}' = 0 (25)$$

$$m_{3,4} - m'_{3,4} = 0. (26)$$

Adding the left sides and right sides of relations (18)-(26), we obtain

$$\sum_{\substack{1 \le i \le j \le 4}} m_{i,j} - \sum_{\substack{1 \le i \le j \le 4}} m'_{i,j} = (-54 + 54k) + (27 - 27k) + (2 - 2k) + (27 - 27k) + (4k - 4) = 2k - 2.$$
(27)

Since

$$n - 1 = \sum_{1 \le i \le j \le 4} m_{i,j} = \sum_{1 \le i \le j \le 4} m'_{i,j}$$

it follows from (27) that k = 1. Thus, from relations (18)-(22),

$$m_{3,3} = m'_{3,3} \quad m_{4,4} = m'_{4,4} \quad m_{2,4} = m'_{2,4} m_{2,2} = m'_{2,2} \quad m_{1,2} = m'_{1,2}.$$
(28)

Finally, from (14) and (28),

$$m\left(T\right) = m\left(T'\right)$$

3 Conditions which assure the weakly discrimination property on an arbitrary class

In our next result we give conditions on a VDB topological index which assures the weakly discrimination property over an arbitrary class $\mathcal{H} \subseteq \mathcal{G}_n$.

Theorem 3.1 Let $\varphi \in \mathbb{R}^h$ be a VDB topological index defined over $\mathcal{H} \subseteq \mathcal{G}_n$ such that $\{\varphi_{i,j}\}_{(i,j)\in K}$ is a linearly independent set over \mathbb{Z} , the set of integers. Then φ is weakly discriminating over \mathcal{H} .

Proof. Let $H, H' \in \mathcal{H}$ and assume that $\varphi(H) = \varphi(H')$. Then

$$0 = (m(H) - m(H')) \cdot \varphi = \sum_{(i,j) \in K} (m_{i,j}(H) - m_{i,j}(H')) \varphi_{i,j}$$

Since $m_{i,j}(H) - m_{i,j}(H') \in \mathbb{Z}$ for all $(i,j) \in K$ and $\{\varphi_{i,j}\}_{(i,j)\in K}$ is a linearly independent set over \mathbb{Z} , $m_{i,j}(H) - m_{i,j}(H') = 0$ for all $(i,j) \in K$. Consequently, m(H) = m(H').

Remark 3.2 The converse of Theorem 3.1 does not hold. For instance, the Sombor index is weakly discriminating over CT_n . However, the components $SO_{2,2}$, $SO_{3,3}$, and $SO_{4,4}$ are $2\sqrt{2}$, $3\sqrt{2}$, and $4\sqrt{2}$, respectively. Note that

$$3SO_{2,2} + 2SO_{3,3} + (-3)SO_{4,4} = 0,$$

so the components of SO are not linearly independent over \mathbb{Z} .

Besicovitch's Theorem can be used to construct many examples of VDB topological indices that are weakly discriminating over $\mathcal{H} \subseteq \mathcal{G}_n$.

Theorem 3.3 [4] (Besicovitch) Let n > 1 be any integer and p_1, \ldots, p_k distinct positive prime numbers. The set of n^k radicals,

$$\left\{\sqrt[n]{p_1^{m(1)} p_2^{m(2)} \cdots p_k^{m(k)}} : 0 \le m(i) < n, \ 1 \le i \le k\right\},\$$

is linearly independent over \mathbb{Z} .

Example 3.4 Consider the sum-connectivity Gourava index $\varphi \in \mathbb{R}^9$ induced by the symmetric function $\varphi(x, y) = \frac{1}{\sqrt{x+y+xy}}$ [14]. Then φ is weakly discriminating over \mathcal{CT}_n . In fact,

$$\varphi = \left(\frac{\sqrt{5}}{5}, \frac{\sqrt{7}}{7}, \frac{1}{3}, \frac{\sqrt{2}}{4}, \frac{\sqrt{11}}{11}, \frac{\sqrt{2 \times 7}}{14}, \frac{\sqrt{3 \times 5}}{15}, \frac{\sqrt{19}}{19}, \frac{\sqrt{2 \times 3}}{12}\right)$$

It follows easily from Besicovitch's Theorem that the set of components of φ is a linearly independent set over \mathbb{Z} , and by Theorem 3.1, the sum-connectivity Gourava index is weakly discriminating over \mathcal{CT}_n .

Based on Besicovitch's Theorem we can introduce weakly discriminating topological indices over arbitrary classes $\mathcal{H} \subseteq \mathcal{G}_n$.

Definition 3.5 The prime topological index is defined as follows: let $\mathcal{H} \subseteq \mathcal{G}_n$, $\Delta = \max \{\Delta(H) : H \in \mathcal{H}\}$ and $h = \frac{\Delta(\Delta+1)}{2}$. Consider the sequence of the first h prime numbers $\{p_{i,j}\}_{(i,j)\in K}$. Then we define the VDB topological index $\Pi = \{\sqrt{p_{i,j}}\}_{(i,j)\in K} \in \mathbb{R}^h$.

Clearly, by Besicovitch's Theorem and Theorem 3.1, Π is weakly discriminating over $\mathcal H.$

Example 3.6 If \mathcal{H} is the set of chemical trees, then $\Pi \in \mathbb{R}^9$ is the vector

$$\Pi = \left(\sqrt{2}, \sqrt{3}, \sqrt{5}, \sqrt{7}, \sqrt{11}, \sqrt{13}, \sqrt{17}, \sqrt{19}, \sqrt{23}\right)$$

and for a chemical tree U,

$$\Pi (U) = \sqrt{2}m_{1,2} + \sqrt{3}m_{1,3} + \sqrt{5}m_{1,4} + \sqrt{7}m_{2,2} + \sqrt{11}m_{2,3} + \sqrt{13}m_{2,4} + \sqrt{17}m_{3,3} + \sqrt{19}m_{3,4} + \sqrt{23}m_{4,4}.$$

We next show how to construct weakly discriminating VDB topological indices φ over $\mathcal{H} \subseteq \mathcal{G}_n$, when all the components of the vector φ are different. First we recall a classical result from algebra. Let \mathcal{A} be the field of algebraic numbers.

Theorem 3.7 [2] (Lindemann-Weierstrass's Theorem) If $\alpha_1, \ldots, \alpha_n$ are distinct algebraic numbers, then $e^{\alpha_1}, \ldots, e^{\alpha_n}$ are linearly independent over \mathcal{A} .

In [19], the exponential of a VDB topological index $\varphi \in \mathbb{R}^h$ over $\mathcal{H} \subseteq \mathcal{G}_n$ was defined for $H \in \mathcal{H}$ as

$$e^{\varphi}(H) = m(H) \cdot e^{\varphi},$$

where $e^{\varphi} \in \mathbb{R}^h$ has components $\{e^{\varphi_{i,j}}\}_{(i,j)\in K}$.

Theorem 3.8 Let $\varphi \in \mathbb{R}^h$ be a VDB topological index defined over $\mathcal{H} \subseteq \mathcal{G}_n$ such that all components of φ are distinct algebraic numbers. Then e^{φ} is weakly discriminating over $\mathcal{H} \subseteq \mathcal{G}_n$.

Proof. Since $\{\varphi_{i,j}\}_{(i,j)\in K}$ are distinct algebraic numbers, it follows from Theorem 3.7 that $\{e^{\varphi_{i,j}}\}_{(i,j)\in K}$ are linearly independent over \mathcal{A} . But $\mathbb{Z} \subseteq \mathcal{A}$. Hence $\{e^{\varphi_{i,j}}\}_{(i,j)\in K}$ are linearly independent over \mathbb{Z} , and the result follows from Theorem 3.1.

Example 3.9 The components of the Sombor index over CT_n are distinct algebraic numbers:

$$SO = \left(\sqrt{5}, \sqrt{10}, \sqrt{17}, 2\sqrt{2}, \sqrt{13}, 2\sqrt{5}, 3\sqrt{2}, 5, 4\sqrt{2}\right).$$

It follows from Theorem 3.8 that e^{SO} is weakly discriminating over \mathcal{CT}_n .

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