

# A Finite-Dimensional Linear Framework for Vertex-Degree-Based Topological Indices

Juan Rada

*Instituto de Matemáticas, Universidad de Antioquia, Medellín, Colombia*

pablo.rada@udea.edu.co

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## Abstract

Vertex-degree-based (VDB) topological indices assign to each edge a weight depending only on the degrees of its endpoints. We develop a unified linear and geometric framework for studying these indices on graph classes with bounded maximum degree.

By encoding each graph through its edge-type vector, every VDB index becomes a linear functional on a finite dimensional space. The analytic form of the generating function plays no essential role: a VDB index is completely determined by its values on degree pairs, and we show that every such index coincides with one induced by a symmetric polynomial. An explicit construction is given for the Sombor index.

We then study discrimination. Strong discrimination is infeasible for VDB indices on several natural graph classes, but a weaker and meaningful notion—weak discrimination—admits a clean linear characterization in terms of the difference space induced by edge-type variations. This leads to general criteria based on support restrictions and linear independence of the weights over  $\mathbb{Q}$ , covering forbidden edge types as well as other structural constraints.

Finally, we investigate extremal values using the feasible polytope generated by edge-type vectors. Maximizers and minimizers of a VDB index correspond to normal cones of this polytope, providing a geometric explanation for the frequent appearance of stars and paths as extremal trees. Several explicit examples illustrate the framework.

# 1 Introduction

Vertex-degree-based (VDB) topological indices are graph invariants defined from a bivariate symmetric function

$$f : [0, +\infty)^2 \rightarrow \mathbb{R}.$$

Given a graph  $G$  with vertex degrees  $d(v)$  and edge set  $E(G)$ , the associated VDB index is defined by

$$I_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)).$$

Thus, each edge contributes a weight depending only on the degrees of its endpoints. This family includes many classical and widely studied indices, such as the Randić index, the Zagreb indices, and the Sombor index, among others.

Two basic questions arise naturally in the study of VDB indices:

- (i) *Discrimination*: to what extent can a given index distinguish non-isomorphic graphs within a fixed class?
- (ii) *Extremality*: within a given class, which graphs maximize or minimize the index?

Both problems have been investigated from different perspectives. Early work on highly discriminating invariants includes Balaban's index [2], and later information-based or polynomial-based approaches were developed in [9–14]. For VDB indices in particular, the notion of *weak discrimination* was introduced in [17], where exponential vertex-degree-based indices were shown to possess strong discriminating properties.

Extremal problems for VDB indices have also received considerable attention, especially in recent work on the Sombor index [1, 3, 5, 7, 8, 16]. Related extremal results for exponential-type VDB indices can be found in [4, 6, 15, 17, 18].

A central point of this paper is that both discrimination and extremal questions become more transparent once vertex-degree-based indices are

placed in a common linear framework. To this end, we encode each graph  $G$  by its *edge-type vector*  $m(G)$ , which records how many edges join vertices of each degree pair. If we collect the values of the defining function  $f$  into a vector

$$\gamma = (f(i, j)),$$

indexed by all admissible degree pairs, then the value of the VDB index can be written in the simple form

$$I_f(G) = \langle \gamma, m(G) \rangle,$$

where  $\langle \cdot, \cdot \rangle$  denotes the Euclidean inner product. Thus every vertex-degree-based index is a linear functional acting on the edge-type vector.

This representation separates two aspects: understanding which edge-type vectors can occur in a given graph class, and understanding how the chosen weights act on those vectors. It also leads naturally to polyhedral methods: extremal graphs correspond to vertices of the convex hull of all edge-type vectors in the class, and the family of indices for which a given graph is extremal is described by the normal cone at the corresponding vertex.

The article is organized as follows. In Section 2 we develop the linear framework based on edge-type vectors and show that the analytic form of the defining function  $f$  is irrelevant: on graph classes with bounded maximum degree, a VDB index is completely determined by its values on degree pairs. This point is further supported by showing that any assignment of weights on degree pairs can be realized by a symmetric polynomial in two variables, and we illustrate this construction with the Sombor index.

Section 3 concerns discrimination. We explain why strong discrimination is unattainable for VDB indices on several natural graph classes and focus instead on weak discrimination. Using the difference space spanned by edge-type variations, we obtain linear criteria for weak discrimination based on support restrictions and  $\mathbb{Q}$ -linear independence of the weights, unifying and extending previous approaches.

In Section 4 we study extremal values of VDB indices from a geometric point of view. We introduce the feasible polytope generated by all edge-type vectors in a given class and show that maximizers and minimizers correspond to normal cones of this polytope. This framework provides a conceptual explanation for the frequent appearance of stars and paths as extremal graphs and is illustrated with explicit small examples.

Overall, the edge-type representation provides a simple and unified setting in which discrimination and extremal problems for vertex-degree-based indices can be studied using linear and geometric tools.

## 2 VDB indices as linear functionals

VDB indices admit a natural linear structure once graphs are encoded through their edge-type vectors. The aim of this section is to make this linearity precise and to show that, on any graph class with bounded maximum degree, every VDB index can be viewed as a linear functional on a finite-dimensional space. We also explain how arbitrary systems of edge weights can be realized by symmetric polynomials, providing an algebraic representation that places all VDB indices within a unified framework.

### 2.1 Edge-type framework and linearity of VDB indices

We begin by fixing the combinatorial space on which VDB indices act linearly. Let  $\mathcal{C}$  be a class of graphs on  $n$  vertices whose vertex degrees lie in  $\{1, \dots, \Delta\}$ ; formally, one may take  $\Delta = n - 1$ , so that the framework applies to all graphs on  $n$  vertices.

Define

$$S_{\Delta} = \{(i, j) : 1 \leq i \leq j \leq \Delta\}, \quad h = |S_{\Delta}| = \Delta(\Delta + 1)/2.$$

The set  $S_{\Delta}$  indexes all possible unordered degree pairs that may occur at the ends of an edge.

For any graph  $G \in \mathcal{C}$ , we define its *edge-type vector*

$$m(G) = (m_{ij}(G))_{(i,j) \in S_\Delta} \in \mathbb{Z}^h,$$

where  $m_{ij}(G)$  denotes the number of edges  $uv \in E(G)$  such that

$$\{d(u), d(v)\} = \{i, j\}.$$

The vector  $m(G)$  records the edge-degree distribution of  $G$  and is invariant under graph isomorphism.

This encoding provides a convenient linearization of the problem: once a graph is represented by its edge-type vector, vertex-degree-based indices can be treated as linear functionals acting on  $m(G)$ .

To make this explicit, let  $f : [0, +\infty)^2 \rightarrow \mathbb{R}$  be any bivariate symmetric function, and define its associated *weight vector*

$$\gamma_f = (\gamma_{ij})_{(i,j) \in S_\Delta} \in \mathbb{R}^h, \quad \gamma_{ij} = f(i, j).$$

Then the VDB index induced by  $f$  can be written as

$$I_f(G) = \langle \gamma_f, m(G) \rangle,$$

where  $\langle \cdot, \cdot \rangle$  denotes the Euclidean inner product on  $\mathbb{R}^h$ .

In particular, two symmetric functions that agree on  $S_\Delta$  induce the same VDB index on  $\mathcal{C}$ .

## 2.2 Polynomial realization of arbitrary weight systems

Although vertex-degree-based indices are defined analytically through a function  $f(i, j)$ , the linear framework introduced above shows that only the finite set of values on degree pairs matters. For several purposes it is therefore convenient to have an explicit algebraic realization of arbitrary weight systems. The following interpolation result provides exactly this: it shows that any assignment of weights on degree pairs can be realized by

a symmetric polynomial in two variables.

**Theorem 1.** *Given an arbitrary collection of real numbers*

$$\{\gamma_{ij} \in \mathbb{R} : (i, j) \in S_\Delta\},$$

*there exists a symmetric polynomial  $Q(x, y) \in \mathbb{R}[x, y]$  such that*

$$Q(i, j) = \gamma_{ij} \quad \text{for all } (i, j) \in S_\Delta.$$

*Proof.* Let  $D = \{1, 2, \dots, \Delta\}$  and let  $L_1, \dots, L_\Delta \in \mathbb{R}[x]$  be the univariate Lagrange polynomials on  $D$ , characterized by  $L_i(k) = \delta_{ik}$ . Define

$$P(x, y) = \sum_{i=1}^{\Delta} \sum_{j=1}^{\Delta} a_{ij} L_i(x) L_j(y),$$

where

$$a_{ij} = \begin{cases} \gamma_{ij}, & i \leq j, \\ \gamma_{ji}, & i > j. \end{cases}$$

Then  $P(k, \ell) = \gamma_{k\ell}$  for all  $(k, \ell) \in S_\Delta$ , and these values extend symmetrically to all of  $D^2$ .

Now define

$$Q(x, y) = \frac{P(x, y) + P(y, x)}{2}.$$

The polynomial  $Q$  is symmetric and satisfies  $Q(i, j) = \gamma_{ij}$  for all  $(i, j) \in S_\Delta$ , as required. ■

An immediate consequence of the above theorem is the following.

**Corollary 1.** *Every vertex-degree-based index on graphs with maximum degree at most  $\Delta$  coincides with an index induced by a symmetric polynomial in two variables.*

### 2.3 Polynomial representation of the Sombor index

We illustrate the interpolation result from the previous subsection by applying it to a concrete and widely studied vertex-degree-based index, namely the Sombor index [16].

**Example 1.** Consider the Sombor index

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2},$$

which is a vertex-degree-based index with weights

$$\gamma_{ij} = \sqrt{i^2 + j^2}.$$

For chemical graphs the maximum degree is  $\Delta = 4$ , so

$$S_4 = \{(i, j) : 1 \leq i \leq j \leq 4\}, \quad D = \{1, 2, 3, 4\}.$$

By Theorem 1, there exists a symmetric polynomial  $Q(x, y)$  such that

$$Q(i, j) = \gamma_{ij} \quad \text{for all } (i, j) \in S_4.$$

**Construction.** Let  $L_1, \dots, L_4$  be the Lagrange polynomials on  $D = \{1, 2, 3, 4\}$ , given by

$$L_1(x) = -\frac{1}{6}(x-2)(x-3)(x-4),$$

$$L_2(x) = \frac{1}{2}(x-1)(x-3)(x-4),$$

$$L_3(x) = -\frac{1}{2}(x-1)(x-2)(x-4),$$

$$L_4(x) = \frac{1}{6}(x-1)(x-2)(x-3).$$

Define

$$Q(x, y) = \sum_{i=1}^4 \sum_{j=1}^4 \gamma_{ij} L_i(x) L_j(y).$$

Since the Sombor weights satisfy  $\gamma_{ij} = \gamma_{ji}$ , the polynomial  $Q$  is symmetric and satisfies

$$Q(i, j) = \sqrt{i^2 + j^2} \quad \text{for all } (i, j) \in S_4.$$

Consequently, on chemical graphs the Sombor index coincides with the

polynomial VDB index induced by  $Q$ , that is,

$$SO(G) = \sum_{uv \in E(G)} Q(d(u), d(v)).$$

The linear representation developed in this section provides a natural starting point for studying discrimination of vertex-degree-based indices. Since every such index acts as a linear functional on the edge-type vector, the question of whether two graphs can be distinguished reduces to analyzing when different edge-type vectors can yield the same inner product value. This observation motivates the study of weak discrimination in the next section.

### 3 Discrimination of VDB topological indices

A fundamental question in the study of topological indices is the extent to which a given invariant can distinguish non-isomorphic graphs. In this section we address this question for VDB indices. We begin by explaining why strong discrimination is unattainable for VDB indices on several natural graph classes. This motivates the introduction of a weaker but more appropriate notion, known as *weak discrimination*, which captures exactly the level of distinction that VDB indices are capable of providing.

#### 3.1 Strong and weak discrimination for VDB indices

A natural ideal for a topological index is to determine the graph uniquely. Formally, an index  $I(G)$  is said to exhibit *strong discrimination* on a graph class  $\mathcal{C}$  if

$$I(G) = I(G') \implies G \cong G' \quad \text{for all } G, G' \in \mathcal{C}.$$

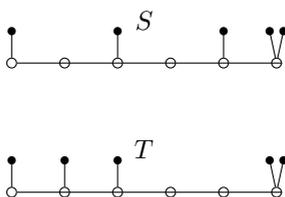
In this case, equal index values force the graphs to be isomorphic.

However, strong discrimination is unattainable for vertex-degree-based (VDB) indices on several natural classes, including chemical trees. The

obstruction is simple: a VDB index depends only on the edge-type vector

$$m(G) = (m_{ij}(G))_{(i,j) \in S_\Delta},$$

and therefore any two graphs with the same edge-type vector necessarily receive the same value under *every* VDB index. In particular, there exist non-isomorphic chemical trees with identical edge-type vectors, as illustrated in Figure 1, and hence identical values for all VDB indices. By attaching the same pendent path to both trees, one obtains such counterexamples with arbitrarily many vertices.



**Figure 1.** Non-isomorphic chemical trees  $S$  and  $T$  with identical edge-type vectors, and hence identical values of all VDB indices.

Since strong discrimination is impossible on these classes, it is natural to consider a weaker notion that still captures meaningful structural insight. Because every VDB index can be written in the linear form

$$I_\gamma(G) = \langle \gamma, m(G) \rangle,$$

a natural relaxation is to require equal index values to force equality of edge-type vectors. This leads to the notion of *weak discrimination*.

### 3.2 Weak discrimination and the difference space

As discussed above, strong discrimination is unattainable for VDB indices on several natural graph classes. A natural relaxation is therefore to require that equal index values force equality of edge-type vectors rather than graph isomorphism.

**Definition 1.** [17] Let  $\mathcal{C}$  be a class of graphs of fixed order  $n$ , and let  $I_\gamma(G) = \langle \gamma, m(G) \rangle$  be a vertex-degree-based index. We say that  $I_\gamma$  is

weakly discriminating on  $\mathcal{C}$  if for all  $G, G' \in \mathcal{C}$ ,

$$I_\gamma(G) = I_\gamma(G') \implies m(G) = m(G').$$

To analyze this property, it is convenient to describe how edge-type vectors can vary within the class. For graphs  $G, G' \in \mathcal{C}$ , define the *difference vector*

$$x(G, G') = m(G') - m(G) \in \mathbb{Z}^h.$$

The rational subspace spanned by all such differences,

$$W(\mathcal{C}) = \text{span}_{\mathbb{Q}}\{m(G') - m(G) : G, G' \in \mathcal{C}\} \subseteq \mathbb{Q}^h,$$

is called the *difference space* of  $\mathcal{C}$ .

The difference space provides a simple way to express weak discrimination in purely linear terms.

**Theorem 2.** *Let  $\mathcal{C}$  be a class of graphs of fixed order  $n$ , and let  $I_\gamma(G) = \langle \gamma, m(G) \rangle$  be a vertex-degree-based index. If*

$$W(\mathcal{C}) \cap \ker \langle \gamma, \cdot \rangle = \{0\},$$

*then  $I_\gamma$  is weakly discriminating on  $\mathcal{C}$ .*

*Proof.* Let  $G, G' \in \mathcal{C}$  and suppose that

$$I_\gamma(G) = I_\gamma(G').$$

Then

$$\langle \gamma, m(G') - m(G) \rangle = 0,$$

so the difference vector  $x = m(G') - m(G)$  belongs to  $\ker \langle \gamma, \cdot \rangle$ . By definition,  $x \in W(\mathcal{C})$ . The hypothesis therefore implies  $x = 0$ , and hence  $m(G) = m(G')$ . This is precisely the definition of weak discrimination. ■

The condition in Theorem 2 is sufficient but not necessary for weak discrimination. The following example shows that a VDB index may be weakly discriminating even when  $W(\mathcal{C}) \cap \ker \langle \gamma, \cdot \rangle$  is nontrivial.

**Example 2.** Let  $\mathcal{C} = \{C_4, P_4, S_4\}$ , the cycle, path, and star on 4 vertices. Here  $\Delta = 3$  and we use the coordinate order

$$(m_{11}, m_{12}, m_{13}, m_{22}, m_{23}, m_{33}).$$

Then

$$m(C_4) = (0, 0, 0, 4, 0, 0); \quad m(P_4) = (0, 2, 0, 1, 0, 0); \quad m(S_4) = (0, 0, 3, 0, 0, 0).$$

Let  $\gamma = (0, 1, -1, 0, 0, 0)$ . Then

$$I_\gamma(C_4) = 0, \quad I_\gamma(P_4) = 2, \quad I_\gamma(S_4) = -3.$$

In particular,  $I_\gamma$  takes distinct values on the three graphs in  $\mathcal{C}$ , so it is weakly discriminating on  $\mathcal{C}$ .

However, the condition in Theorem 2 fails. Indeed, the vector

$$w = (0, 6, 6, -17, 0, 0) = 3(m(P_4) - m(C_4)) + 2(m(S_4) - m(C_4))$$

belongs to  $W(\mathcal{C})$  and satisfies

$$\langle \gamma, w \rangle = 6 - 6 = 0.$$

Thus  $0 \neq w \in W(\mathcal{C}) \cap \ker\langle \gamma, \cdot \rangle$ , showing that  $W(\mathcal{C}) \cap \ker\langle \gamma, \cdot \rangle = \{0\}$  is not necessary for weak discrimination.

### 3.3 Support-restricted subspaces and independence of coefficients

To apply the linear criterion efficiently, it is useful to control the support of difference vectors. For a subset  $S \subseteq S_\Delta$ , define the coordinate subspace

$$U_S = \{x \in \mathbb{Q}^h : x_{ij} = 0 \text{ for all } (i, j) \notin S\}.$$

Thus  $U_S$  consists of all vectors whose nonzero coordinates are indexed by  $S$ .

The following result shows that weak discrimination follows whenever the difference space is contained in such a coordinate subspace and the corresponding coefficients are linearly independent.

**Theorem 3.** *Let  $\mathcal{C}$  be a class of graphs with maximum degree  $\Delta$ , and let  $S \subseteq S_\Delta$ . If*

$$W(\mathcal{C}) \subseteq U_S$$

*and the weights  $\{\gamma_{ij} : (i, j) \in S\}$  are linearly independent over  $\mathbb{Q}$ , then the vertex-degree-based index  $I_\gamma$  is weakly discriminating on  $\mathcal{C}$ .*

*Proof.* Let  $G, G' \in \mathcal{C}$  and suppose that

$$I_\gamma(G) = I_\gamma(G').$$

Then

$$\langle \gamma, m(G') - m(G) \rangle = 0.$$

Since  $m(G') - m(G) \in W(\mathcal{C}) \subseteq U_S$ , we obtain

$$0 = \sum_{(i,j) \in S} \gamma_{ij} (m_{ij}(G') - m_{ij}(G)).$$

By the  $\mathbb{Q}$ -linear independence of the coefficients  $\{\gamma_{ij} : (i, j) \in S\}$ , it follows that

$$m_{ij}(G') - m_{ij}(G) = 0 \quad \text{for all } (i, j) \in S.$$

Hence  $m(G) = m(G')$ , and  $I_\gamma$  is weakly discriminating on  $\mathcal{C}$ . ■

In many graph classes the inclusion  $W(\mathcal{C}) \subseteq U_S$  arises from simple structural constraints, such as the absence of certain edge types.

### 3.4 Forbidden edge types

The support condition  $W(\mathcal{C}) \subseteq U_S$  often follows from simple structural restrictions on the graph class. A common situation is when certain edge types never occur in the graphs of the class. Let  $F \subseteq S_\Delta$  be a set of *forbidden edge types* in  $\mathcal{C}$ , that is, edge types that never appear in the

graphs of the class. Thus

$$m_{ij}(G) = 0 \quad \text{for all } (i, j) \in F \text{ and all } G \in \mathcal{C}.$$

Set  $S = S_\Delta \setminus F$ .

**Corollary 2.** *Let  $\mathcal{C}$  be a class of graphs with maximum degree  $\Delta$ , and let  $F \subseteq S_\Delta$  be a forbidden set of edge types. If the weights  $\{\gamma_{ij} : (i, j) \in S\}$  are linearly independent over  $\mathbb{Q}$ , where  $S = S_\Delta \setminus F$ , then the vertex-degree-based index  $I_\gamma$  is weakly discriminating on  $\mathcal{C}$ .*

*Proof.* If  $(i, j) \in F$  and  $G, G' \in \mathcal{C}$ , then  $m_{ij}(G) = m_{ij}(G') = 0$ . Hence every difference vector  $m(G') - m(G)$  has zero coordinates in all positions indexed by  $F$ , and therefore  $W(\mathcal{C}) \subseteq U_S$  with  $S = S_\Delta \setminus F$ . The conclusion follows from Theorem 3. ■

This corollary is particularly effective when the remaining set  $S$  is small, since it is then easy to choose coefficients that are linearly independent over  $\mathbb{Q}$ . For instance, one may assign

$$\gamma_{ij} = \sqrt{q_{ij}} \quad \text{for } (i, j) \in S,$$

where the  $q_{ij}$  are distinct squarefree positive integers; it is well known that these square roots are linearly independent over  $\mathbb{Q}$ .

The corollary also applies in situations where no edge types are forbidden, provided that the full set of coefficients is arithmetically independent.

**Example 3.** In the setting of Corollary 2, consider the case in which no edge types are forbidden, that is,  $F = \emptyset$  and hence  $S = S_\Delta$ . Let  $\{\lambda_{ij} : (i, j) \in S_\Delta\}$  be distinct algebraic numbers and define the exponential vertex-degree-based index

$$I_\lambda(G) = \sum_{(i,j) \in S_\Delta} e^{\lambda_{ij}} m_{ij}(G).$$

By the Lindemann–Weierstrass theorem, the numbers  $\{e^{\lambda_{ij}} : (i, j) \in S_\Delta\}$  are linearly independent over  $\mathbb{Q}$ . Therefore the coefficient vector  $\gamma =$

$(e^{\lambda_{ij}})_{(i,j) \in S_\Delta}$  satisfies the hypothesis of Corollary 2, and  $I_\lambda$  is weakly discriminating on  $\mathcal{C}$ .

A typical application of Corollary 2 arises in chemical graph theory.

**Example 4.** Catacondensed hexagonal systems form a well-studied class of benzenoid graphs. For a fixed number of hexagons, all graphs in this class have the same number of vertices, and every vertex has degree 2 or 3.

Writing

$$S_3 = \{(i, j) : 1 \leq i \leq j \leq 3\},$$

it follows that the edge types

$$(1, 1), (1, 2), (1, 3)$$

are forbidden in this class. Hence

$$m_{1,1}(G) = m_{1,2}(G) = m_{1,3}(G) = 0 \quad \text{for all } G \in \mathcal{C}.$$

In the notation of Corollary 2, we may take

$$F = \{(1, 1), (1, 2), (1, 3)\}, \quad S = S_3 \setminus F = \{(2, 2), (2, 3), (3, 3)\}.$$

By Corollary 2, any vertex-degree-based index

$$I_\gamma(G) = \langle \gamma, m(G) \rangle$$

for which the weights  $\{\gamma_{22}, \gamma_{23}, \gamma_{33}\}$  are linearly independent over  $\mathbb{Q}$  is weakly discriminating on the class of catacondensed hexagonal systems.

It is worth emphasizing that the support restriction  $W(\mathcal{C}) \subseteq U_S$  may also arise when no edge types are forbidden. Indeed, certain edge-type coordinates may be structurally forced to be constant across the class and therefore vanish in all difference vectors.

**Example 5.** Fix an integer  $p \geq 2$  and consider the class  $\mathcal{C}_p$  of chemical trees satisfying:

1. there are exactly  $p$  vertices of degree 4;
2. each degree-4 vertex is adjacent to three leaves and to exactly one vertex of degree 2.

Each degree-4 vertex contributes three edges of type (1, 4) and one edge of type (2, 4). Since there are  $p$  such vertices in every  $G \in \mathcal{C}_p$ , we have

$$m_{1,4}(G) = 3p, \quad m_{2,4}(G) = p, \quad \text{for all } G \in \mathcal{C}_p.$$

Thus the coordinates  $m_{1,4}$  and  $m_{2,4}$  are constant on  $\mathcal{C}_p$ , and for any  $G, G' \in \mathcal{C}_p$  the difference vector  $m(G') - m(G)$  satisfies

$$(m(G') - m(G))_{1,4} = 0, \quad (m(G') - m(G))_{2,4} = 0.$$

Equivalently,

$$W(\mathcal{C}_p) \subseteq U_S, \quad S = S_4 \setminus \{(1, 4), (2, 4)\}.$$

Although the edge types (1, 4) and (2, 4) are not forbidden, they do not appear in any difference vector, since their corresponding coordinates are constant on  $\mathcal{C}_p$ . Consequently, Theorem 3 applies directly and yields weak discrimination for all VDB indices whose weights  $\{\gamma_{ij} : (i, j) \in S\}$  are linearly independent over  $\mathbb{Q}$ .

## 4 Extremal values of VDB indices: a geometric viewpoint

To study extremal values of vertex-degree-based indices, we adopt a geometric point of view based on convex polytopes; see, for instance, [19] for background.

A convex polytope in  $\mathbb{R}^h$  is the convex hull of a finite set  $X \subset \mathbb{R}^h$ , that is,

$$P = \text{conv}(X) = \left\{ \sum_{k=1}^r \lambda_k x_k : r \geq 1, x_k \in X, \lambda_k \geq 0, \sum_{k=1}^r \lambda_k = 1 \right\}.$$

A point  $x \in P$  is called a *vertex* (or *extreme point*) of  $P$  if it cannot be written as a nontrivial convex combination of two distinct points of  $P$ . We denote the set of all vertices of  $P$  by  $\text{vert}(P)$ .

Let  $\mathcal{C}$  be a graph class and consider the finite set of edge-type vectors

$$M(\mathcal{C}) = \{m(G) : G \in \mathcal{C}\} \subset \mathbb{R}^h.$$

Its convex hull

$$P = \text{conv}(M(\mathcal{C}))$$

will be called the *feasible polytope* of the class. Since  $M(\mathcal{C})$  is finite,  $P$  is a polytope, and each of its vertices corresponds to the edge-type vector of one or more graphs in  $\mathcal{C}$ .

Because every VDB index has the linear form

$$I_\gamma(G) = \langle \gamma, m(G) \rangle,$$

maximizing or minimizing  $I_\gamma$  over  $\mathcal{C}$  is equivalent to maximizing or minimizing the linear functional  $\langle \gamma, \cdot \rangle$  over  $P$ . Consequently, all extremal values of  $I_\gamma$  are attained at vertices of  $P$ , and the determination of extremal graphs reduces to the study of the normal cones of these vertices.

## 4.1 Maximizing a VDB index on a graph class

Fix a class of graphs  $\mathcal{C}$  and a weight vector  $\gamma$ . Maximizing  $I_\gamma$  over  $\mathcal{C}$  is equivalent to maximizing the linear functional  $\langle \gamma, \cdot \rangle$  over the polytope  $P$ :

$$\max_{G \in \mathcal{C}} I_\gamma(G) = \max_{x \in P} \langle \gamma, x \rangle.$$

By polytope theory, the maximum is attained at a vertex of  $P$ , and a vertex  $x \in P$  satisfies

$$x \text{ maximizes } \langle \gamma, \cdot \rangle \text{ on } P \iff \gamma \in N_P(x),$$

where the normal cone at  $x$  is

$$N_P(x) = \{\gamma : \langle \gamma, y - x \rangle \leq 0 \text{ for all } y \in P\}.$$

If  $\gamma$  lies in the interior of  $N_P(x)$ , then  $x$  is the unique maximizer.

The corresponding statement for minimizers follows by replacing  $\gamma$  with  $-\gamma$ :

$$x \text{ minimizes } \langle \gamma, \cdot \rangle \text{ on } P \iff -\gamma \in N_P(x).$$

Moreover,  $x$  is the unique minimizer of  $I_\gamma$  if and only if  $-\gamma$  lies in the interior of  $N_P(x)$ .

In summary, determining the extremal graphs for a VDB index  $I_\gamma$  reduces to locating the weight vector  $\gamma$  inside the normal fan  $\{N_P(x) : x \in \text{vert}(P)\}$  of  $P$ . Maximizers correspond to cones containing  $\gamma$ , and minimizers to cones containing  $-\gamma$ .

In principle, one could determine all vertices of  $P$  and compute their normal cones, thereby solving the extremal problem completely. However,  $P$  is typically very large: even for chemical trees the number of possible edge-type vectors grows rapidly with  $n$ , so determining  $\text{vert}(P)$  explicitly is feasible only for very small classes. Nevertheless, this geometric viewpoint remains powerful, because many important extremal phenomena depend only on a small number of cones of  $P$ .

## 4.2 The dual viewpoint and classical extremal graphs

The same geometric framework also answers the reverse question: given a graph  $G \in \mathcal{C}$ , for which weight vectors  $\gamma$  does  $G$  maximize or minimize the index  $I_\gamma$ ?

Let  $x_G = m(G)$  denote the edge-type vector of  $G$ . Then

$$G \text{ maximizes } I_\gamma \text{ on } \mathcal{C} \iff \gamma \in N_P(x_G),$$

and

$$G \text{ minimizes } I_\gamma \text{ on } \mathcal{C} \iff -\gamma \in N_P(x_G).$$

Thus the normal cone  $N_P(x_G)$  describes precisely the family of vertex-degree-based indices for which  $G$  is a maximizer. Moreover, interior points of this cone correspond to indices for which  $G$  is a *unique* maximizer. A graph  $G$  can be uniquely extremal for some VDB index if and only if  $x_G \in \text{vert}(P)$ ; if  $x_G$  lies on a higher-dimensional face of  $P$ , then  $N_P(x_G)$  has empty interior and no VDB index can single out  $G$  uniquely.

This dual viewpoint provides a transparent explanation for the frequent appearance of the star and the path as extremal graphs for many classical indices. We illustrate this phenomenon for the class  $\mathcal{T}_n$  of all trees on  $n$  vertices.

The star  $S_n$  is the unique tree containing a vertex of degree  $n - 1$ . Its edge-type vector has only one nonzero entry,

$$m(S_n)_{1,n-1} = n - 1, \quad m(S_n)_{i,j} = 0 \text{ otherwise.}$$

Any tree  $G \neq S_n$  necessarily has fewer edges of type  $(1, n - 1)$ . Consequently, for every  $G \neq S_n$ , the difference vector  $m(G) - m(S_n)$  has a positive entry in some coordinate  $(i, j) \neq (1, n - 1)$  where  $m(S_n)$  is zero. It follows that the normal cone

$$N_P(m(S_n)) = \{\gamma : \langle \gamma, m(G) - m(S_n) \rangle \leq 0 \text{ for all } G \in \mathcal{T}_n\}$$

is the full-dimensional cone determined by the inequalities

$$\gamma_{1,n-1} \geq \gamma_{i,j} \quad \text{for all } (i, j) \neq (1, n - 1).$$

Any weight vector  $\gamma$  satisfying these inequalities makes  $S_n$  a maximizer of  $I_\gamma$  on  $\mathcal{T}_n$ , and if the inequalities are strict then  $S_n$  is the unique maximizer.

A completely analogous argument applies to the path  $P_n$ . The degrees of  $P_n$  belong to  $\{1, 2\}$ , and its edge-type vector has nonzero entries only of types  $(1, 2)$  and  $(2, 2)$ . Every other tree contains an edge of type  $(i, j)$  with  $j \geq 3$ , and hence

$$N_P(m(P_n)) = \{\gamma : \gamma_{1,2} \leq \gamma_{i,j}, \gamma_{2,2} \leq \gamma_{i,j} \text{ for all } (i, j) \notin \{(1, 2), (2, 2)\}\}.$$

Thus any weight vector  $\gamma$  that assigns larger weights to higher-degree edges lies in the normal cone of  $P_n$ , making the path the unique minimizer of  $I_\gamma$  on  $\mathcal{T}_n$ .

**Consequences.** These descriptions allow several classical indices to be placed naturally inside these cones. For example:

- The Sombor index has weights  $\gamma_{i,j}^{SO} = \sqrt{i^2 + j^2}$ , which are strictly increasing in  $i+j$ . Hence  $\gamma^{SO} \in \text{int } N_P(m(S_n))$ , and  $S_n$  is the unique maximizer of  $SO$  on  $\mathcal{T}_n$ .
- For the first Zagreb index,  $\gamma_{i,j}^{Z_1} = i+j$ , again strictly increasing in the degrees. Thus  $\gamma^{Z_1} \in \text{int } N_P(m(S_n))$ , and  $S_n$  is the unique maximizer on  $\mathcal{T}_n$ .
- The Randić index  $R_\alpha$  has weights  $\gamma_{i,j} = (ij)^\alpha$ . When  $\alpha < 0$ , the weights decrease as the degrees increase, so  $\gamma \in \text{int } N_P(m(P_n))$  and the path is the unique minimizer.

These examples show that the normal cones  $N_P(m(S_n))$  and  $N_P(m(P_n))$  contain large regions of  $\mathbb{R}^h$ . This explains why the star and the path repeatedly appear as extremal graphs for a wide variety of vertex-degree-based indices.

### 4.3 Illustrative examples

The geometric machinery developed above is completely general, but it becomes most transparent when applied to small graph classes for which the feasible polytope  $P = \text{conv}(M(C))$  and its normal cones can be computed explicitly. We present two such examples, which already illustrate the fundamental mechanisms underlying extremal values of vertex-degree-based indices.

**Example 6.** Consider  $\mathcal{T}_4 = \{P_4, S_4\}$ , the set of trees with four vertices. Their edge-type vectors in the coordinate system

$$(m_{11}, m_{12}, m_{13}, m_{22}, m_{23}, m_{33})$$

are

$$m(P_4) = (0, 2, 0, 1, 0, 0), \quad m(S_4) = (0, 0, 3, 0, 0, 0).$$

The feasible polytope

$$P = \text{conv}(m(P_4), m(S_4))$$

is a line segment with exactly two vertices. Let  $d = m(P_4) - m(S_4)$ . Then

$$N_P(m(P_4)) = \{\gamma : \langle \gamma, d \rangle \geq 0\}, \quad N_P(m(S_4)) = \{\gamma : \langle \gamma, d \rangle \leq 0\}.$$

Thus  $P_4$  is a maximizer of  $I_\gamma$  for all  $\gamma$  satisfying  $\langle \gamma, d \rangle \geq 0$ , and  $S_4$  is a maximizer when the inequality is reversed.

**Example 7.** Now consider the class of trees with four vertices  $\{C_4, P_4, S_4\}$ . The cycle, path, and star on four vertices have edge-type vectors

$$m(C_4) = (0, 0, 0, 4, 0, 0); \quad m(P_4) = (0, 2, 0, 1, 0, 0); \quad m(S_4) = (0, 0, 3, 0, 0, 0).$$

Thus

$$P = \text{conv}(m(C_4), m(P_4), m(S_4)) \subset \mathbb{R}^6.$$

Since these three points are affinely independent,  $P$  is a 2-dimensional simplex. To compute the normal cones, we form the difference vectors

$$\begin{aligned} p - c &= (0, 2, 0, -3, 0, 0), & s - c &= (0, 0, 3, -4, 0, 0), \\ c - p &= (0, -2, 0, 3, 0, 0), & s - p &= (0, -2, 3, -1, 0, 0), \\ c - s &= (0, 0, -3, 4, 0, 0), & p - s &= (0, 2, -3, 1, 0, 0). \end{aligned}$$

For a vertex  $x$ , the normal cone  $N_P(x)$  is the intersection of the half-spaces  $\langle \gamma, y - x \rangle \leq 0$  corresponding to the two adjacent vertices  $y$ .

Hence

$$N_P(m(C_4)) = \left\{ \gamma : 2\gamma_{12} - 3\gamma_{22} \leq 0, 3\gamma_{13} - 4\gamma_{22} \leq 0 \right\},$$

$$N_P(m(P_4)) = \left\{ \gamma : -2\gamma_{12} + 3\gamma_{22} \leq 0, -2\gamma_{12} + 3\gamma_{13} - \gamma_{22} \leq 0 \right\},$$

$$N_P(m(S_4)) = \left\{ \gamma : -3\gamma_{13} + 4\gamma_{22} \leq 0, 2\gamma_{12} - 3\gamma_{13} + \gamma_{22} \leq 0 \right\}.$$

These three cones partition  $\mathbb{R}^6$  (up to boundaries) and specify exactly which choices of  $\gamma$  make  $C_4$ ,  $P_4$ , or  $S_4$  maximizers of  $I_\gamma$ .

Because minimization of  $\langle \gamma, \cdot \rangle$  is equivalent to maximization of  $\langle -\gamma, \cdot \rangle$ , the cones above also describe all minimizers: a vertex  $x$  is a minimizer of  $I_\gamma$  if and only if  $-\gamma \in N_P(x)$ . Unique minimizers arise exactly when  $-\gamma$  lies in the interior of the corresponding cone.

These examples show how extremal behaviour of vertex–degree–based indices is encoded geometrically in the feasible polytope  $P$  and its normal fan. Although  $P$  is too large to describe explicitly for general graph classes, the geometric viewpoint clarifies the structure of the extremal problem and the reasons behind the prominent role of stars and paths.

## 5 Conclusions

In this paper we developed a linear and geometric framework for the study of VDB indices on graph classes with bounded maximum degree. By encoding graphs through their edge–type vectors, both discrimination and extremal problems can be treated in a unified finite–dimensional setting.

For discrimination, we showed that weak discrimination is determined by the difference space associated with the class. Support restrictions, whether arising from forbidden edge types or from structural constraints that force certain coordinates to be constant, lead to simple and general sufficient conditions for weak discrimination. These results unify several previously known criteria and clarify the role of arithmetic independence of the weights.

For extremal problems, the same encoding leads to a geometric view in terms of linear optimization over a feasible polytope. Extremal graphs correspond to vertices of this polytope, and the families of indices for which a given graph is extremal are described by its normal cones. From this viewpoint, it becomes clear why stars and paths so often arise as extremal graphs for many VDB indices.

Overall, the edge-type representation provides a transparent framework that connects combinatorial structure, arithmetic properties of the weights, and convex geometry. We expect that this approach can be extended to other classes of graphs and to broader families of degree-based invariants.

## References

- [1] S. Ahmad, R. Farooq, K. C. Das, The general Sombor index of extremal trees with a given maximum degree, *MATCH Commun. Math. Comput. Chem.* **94** (2025) 825–853.
- [2] A. T. Balaban, Highly discriminating distance-based topological index, *Chem. Phys. Lett.*, **89** (1982) 399–404.
- [3] M. Chen, Y. Zhu, Extremal unicyclic graphs of Sombor index. *Appl. Math. Comput.*, **463** (2024) #128374.
- [4] K. C. Das, S. Elumalai, S. Balachandran, Open problems on the exponential vertex-degree-based topological indices of graphs, *Discr. Appl. Math.* **293** (2021) 38–49.
- [5] K. C. Das, Open problems on Sombor index of unicyclic and bicyclic graphs, *Appl. Math. Comput.* **473** (2024) #128647.
- [6] K. C. Das, On the exponential atom-bond connectivity index of graphs, *Mathematics* **13** (2025) #269.
- [7] K. C. Das, C. Xu, Proof of a conjecture on Sombor index and the least Sombor eigenvalue of graphs, *MATCH Commun. Math. Comput. Chem.* **94** (2025) 855–862.
- [8] K. C. Das, I. Gutman, A. Ali, Augmented Sombor index, *MATCH Commun. Math. Comput. Chem.* **95** (2026) 523–547.
- [9] M. Dehmer, M. Grabner, K. Varmuza, Information indices with high discriminative power for graphs, *PLoS ONE* **7** (2012) #e31214.

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- [10] M. Dehmer, M. Grabner, A. Mowshowitz, F. Emmert-Streib, An efficient heuristic approach to detecting graph isomorphism based on combinations of highly discriminating invariants. *Adv. Comput. Math.* **39** (2013) 311–325.
- [11] M. Dehmer, A. Mowshowitz, The discrimination power of structural superindices. *PLoS ONE* **8** (2013) #e70551.
- [12] M. Dehmer, Z. Chen, F. Emmert-Streib, Y. Shi, S. Tripathi, Graph measures with high discrimination power revisited: A random polynomial approach, *Inf. Sci.* **467** (2018) 407–414.
- [13] M. V. Diudea, A. Ilić, K. Varmuza, M. Dehmer, Network analysis using a novel highly discriminating topological index, *Complexity* **16** (2011) 32–39.
- [14] T. Došlić, T. Réti, Novel degree-based molecular descriptors with increased discriminating power, *Acta Polytech. Hung.* **9** (2012) 17–30.
- [15] W. Gao, Y. Gao, The extremal trees for exponential vertex-degree-based topological indices, *Appl. Math. Comput.* **472** (2024) #128634.
- [16] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.
- [17] J. Rada, Exponential vertex–degree–based topological indices and discrimination, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 29–41.
- [18] C. Xu, L. Buyantogtokh, S. Dorjsembe, D. Bolormaa, S. Bao, Exponential augmented Zagreb index of  $(n,m)$ -graphs, *Discrete Appl. Math.* **376** (2025) 151–159.
- [19] G. M. Ziegler, *Lectures on Polytopes*, Graduate Texts in Mathematics 152, Springer, 1995.