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A HYBRID TOPOLOGICAL INDEX BASED ON LAPLACIAN AND DISTANCE SPECTRA

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Abstract

In graph theory, the topological indices translate complex combinatorial properties such as connectivity, distances, branching, and symmetry into single quantitative measures. They play a crucial role in comparing graphs, studying extremal structures, analyzing chemical molecules, and developing models in network science. By summarizing key aspects of a graph's topology, the indices provide a powerful tool for both theoretical investigations and real-world applications.

In this paper, the authors introduce a new topological index for finite simple connected graphs which is called as Distance-Spectral Mixed Index (DSMI), that combines two different spectra, the Laplacian and distance spectra. Let G be a connected graph of order n with Laplacian eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \lambda_3 \dots \dots \dots \leq \lambda_n$ and distance-matrix eigenvalues $\mu_1 \geq \mu_2 \geq \mu_3 \dots \dots . \geq \mu_n$. The $DSMI(G)$is defined as $\sum_{k=1}^{n} \frac{\lambda_k}{\mu_k+1}$. The authors discussed the invariance and nonnegativity, upper and lower bounds in terms of classical invariants like order, diameter, algebraic connectivity, established results on monotonicity under elementary graph operations such as addition of edge and vertex, subdivision of edge and the exact values for complete graphs, complete bipartite graphs, paths, and stars are obtained.

1. Introduction

A topological index serves as a numerical descriptor that conveys essential structural properties of a graph without depending on labels or coordinates. Spectral graph invariants have played a vital role in understanding structure of a graph. Traditional indices which are derived from adjacency, Laplacian, or distance matrices, each highlight different structural features of graphs such as connectivity, path or metric properties. Because these matrices reflect complementary aspects of a graph, it is natural to explore indices that combine their strengths

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to capture a more complete description. The Distance Spectral Mixed Index brings together information from the Laplacian spectrum, which relates to connectivity and cut structure, and the distance spectrum, which is reflective of metric properties. The authors approach is entirely theoretical and combinatorial. The goal is to develop rigorous properties, bounds, and extremal behavior for this index without application-based examples.

Our development of a new distance spectral index is motivated by the rich theory of graph spectra documented in classical references such as Brouwer et al. (2012) and Cvetković et al. (2010), as well as modern studies on distance matrices.

Since distance based and spectral invariants play an important role in QSAR/QSPR modeling, as highlighted by Gutman et al. (2004), Estrada (2000) and Dehmer et al. (2009), our DSM construction extends this line of research with a mixed distance Laplacian perspective.

2. Preliminaries and notation

Throughout the paper, $G = (V, E)$ is a finite simple undirected and connected graph with $n \geq 1$ vertices. The Distances $d_G(u, v)$ are the shortest path lengths.

Denote Adjacency matrix as $A(G)$, the degree diagonal matrix as $D_d(G)$, a Laplacian matrix as $L(G) = D_d(G) - A(G)$ which is a symmetric positive semidefinite matrix and the distance matrix as $D(G)$.

The Laplacian eigenvalues are denoted by $0 = \lambda_1 \leq \lambda_2 \leq \lambda_3 \dots \dots \dots \leq \lambda_n$ and distance-matrix eigenvalues are $\mu_1 \geq \mu_2 \geq \mu_3 \dots \dots . \geq \mu_n$.

3. Distance Spectral Mixed Index (DSMI) of a graph

Definition: For a connected graph G with Laplacian eigenvalues $\{\lambda_i\}_{i=1}^{n}$ordered nondecreasing and distance eigenvalues $\{\mu_i\}_{i=1}^{n}$ordered nonincreasing, define

$$\mathrm{DSMI}(G) = \sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1}.$$

Remarks on well-definedness and pairing: Both Laplacian and distance eigenvalue lists are multisets determined by G. The DSMI as defined pairs the i-th smallest Laplacian eigenvalue with the i-th largest distance eigenvalue. One may ask whether this pairing is canonical. This pairing is a specific choice (in practice, one may also pair eigenvalues by index in any consistent ordering; results that depend on the pairing must be stated with that choice). The denominator $\mu_i + 1$is finite because $\mu_i = -(n - 1)$.

If for some i, $\mu_i = -1$, then that single summand is formally undefined. In many standard graph families such as complete graphs, paths, cycles, stars, and complete bipartite graphs, the value $\mu_i = -1$ appears naturally, often with high multiplicity.

Volume 38 No. 12s, 2025

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For example, in the complete graph, the distance eigenvalue −1 occurs with multiplicity n − 1.

To avoid singular behaviour, the authors consider two possible cases in the existence of DSMI of a graph.

Case 1:

$$\mathrm{DSMI}_{\varepsilon}(G)=\sum_{i=1}^{n}\frac{\lambda_i}{\mu_i+1+\varepsilon},$$

and then take limit $\varepsilon \to 0$,

Case 2:

$$\mathrm{DSMI}^{*}(G)=\sum_{i=1}^{n}\frac{\lambda_i}{|\mu_i|+1}$$

In later sections, the authors adopt regularization when necessary and explicitly note where the standard DSMI is finite.

4. Basic Properties and Bounds of DSMI

Theorem 4.1: If $G \cong H$ then $\mathrm{DSMI}(G)=\mathrm{DSMI}(H)$.
Proof: Graph isomorphism corresponds to simultaneous permutation similarity of the adjacency, degree, Laplacian, and distance matrices, preserving their spectra as multisets. Since DSM is a function only of the two ordered eigenvalue lists (with the specified pairing), the value is preserved.

Lemma 4.2: If $G$is connected and $n \geq 1$, then $\mathrm{DSMI}(G) \geq 0$. Moreover, $\mathrm{DSMI}(G)=0$ if and only if $n=1$.
Proof: Each Laplacian eigenvalue $\lambda_i \geq 0$. For $n>1$there exists some $\lambda_j>0$, hence at least one summand is positive (provided the denominator is finite). All denominators are real and finite, thus $\mathrm{DSMI} \geq 0$.

If $n=1$, $L=[0]$, Dist $=[0]$, so $\mathrm{DSMI}=0$.

Conversely, if $\mathrm{DSMI}=0$, then each term must be zero; but $\frac{\lambda_i}{\mu_i+1}=0$, for all i forces each $\lambda_i=0$. So $L=0$. Hence no edges in G and $n=1$.

Proposition 4.3: For every connected graph G,

$$\mathrm{DSMI}(G) \leq \left(\sum_{i=1}^{n}\lambda_i^2\right)^{1/2}\left(\sum_{i=1}^{n}\frac{1}{(\mu_i+1)^2}\right)^{1/2}.$$

Proof. The Immediate application of the Cauchy–Schwarz inequality to sequences $a_i=\lambda_i$and $b_i=\frac{1}{\mu_i+1}$ gives

Volume 38 No. 12s, 2025

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$$\left(\sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1}\right)^2 \le \left(\sum_{i=1}^{n} \lambda_i^2\right)\left(\sum_{i=1}^{n} \frac{1}{(\mu_i + 1)^2}\right).$$

Taking square roots yields the claim.

Corollary 4.4: Using $\sum \lambda_i^2 = \mathrm{trace}(L^2)$, and combinatorial bounds on $\mathrm{trace}(L^2) \le 2m$ (or a tighter $\mathrm{trace}(L^2) = \sum_v d(v)^2 + 2m$ depending on normalization), so a combinatorial upper bound on DSMI is obtained.

Preposition 4.5: For every connected graph G, Let $\lambda_2$be the algebraic connectivity and $\mu_1$the largest distance eigenvalue. Then

$$\mathrm{DSMI}(G) \ge \frac{\lambda_2}{\mu_1 + 1}.$$

Proof: For $i \ge 2$, $\lambda_i \ge \lambda_2$.

For all i, $\mu_i \le \mu_1$, thus $\mu_i + 1 \le \mu_1 + 1$.
Therefore,

$$\frac{\lambda_i}{\mu_i + 1} \ge \frac{\lambda_2}{\mu_1 + 1} \text{for } i \ge 2.$$

Including $i = 1$ with $\lambda_1 = 0$, gives

$$\mathrm{DSMI}(G) = \sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1} \ge \frac{\lambda_2}{\mu_1 + 1}.$$

If $\mu_1 + 1$is negative, the inequality direction reverses and in typical connected graphs $\mu_1 \ge 0$, so the bound makes sense.

Proposition 4.6: Let Gbe a connected graph with Laplacian eigenvalues

$$0 = \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$$

and distance eigenvalues

$$\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n.$$

Let the DSM index be defined as

$$\mathrm{DSMI}\ (G) = \sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1}.$$

Then the DSM index satisfies the upper bound

$$\mathrm{DSMI}\ (G) \le \frac{\mathrm{tr}\ (L)}{\mu_n + 1},$$

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where tr $(L) = \sum_{i=1}^{n} \lambda_i = 2m$ (twice the number of edges) is the trace of the Laplacian matrix and μ_n is the smallest distance eigenvalue.

Proof: Since the Laplacian eigenvalues are nonnegative, we have $\lambda_i \geq 0,$ for all i. Because the distance eigenvalues are ordered nonincreasing, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$, the smallest denominator in the DSMI summand is $\mu_n + 1$. Therefore, for every i,

$$\frac{\lambda_i}{\mu_i + 1} \leq \frac{\lambda_i}{\mu_n + 1},$$

because increasing the denominator decreases the value of the fraction (and all denominators are positive for the graph classes considered).

Summing the above inequality over all $\mathrm{i} = 1, \ldots, \mathrm{n}$, we obtain

$$\mathrm{DSMI}\ (\mathrm{G}) = \sum_{\mathrm{i}=1}^{\mathrm{n}} \frac{\lambda_{\mathrm{i}}}{\mu_{\mathrm{i}} + 1} \leq \sum_{\mathrm{i}=1}^{\mathrm{n}} \frac{\lambda_{\mathrm{i}}}{\mu_{\mathrm{n}} + 1} = \frac{1}{\mu_{\mathrm{n}} + 1} \sum_{\mathrm{i}=1}^{\mathrm{n}} \lambda_{\mathrm{i}}.$$

Recalling that $\sum_{i=1}^{n} \lambda_i = tr\ (L) = 2m$, the number of edges in G

So

$$\boxed{DSM\, I(G) \leq \frac{\mathrm{tr}(L)}{\mu_n + 1}.}$$

Theorem 4.7: Let Gbe a connected graph with Laplacian eigenvalues

$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$$

and distance eigenvalues

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n.$$

Then the DSM index satisfies

$$\mathrm{DSMI}\ (G) \geq \frac{\lambda_2}{\mu_1 + 1} + \frac{\lambda_n}{\mu_n + 1}.$$

Proof: Because the summand

$$f_i = \frac{\lambda_i}{\mu_i + 1}$$

pairs the smallest Laplacian eigenvalues with the largest distance eigenvalues, and vice versa, the extreme contributions arise from the pairs $(\lambda_2, \mu_1)$and (λ_n, μ_n). Since every other eigenvalue pair lies between these extremes, we obtain

Volume 38 No. 12s, 2025

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$$\mathrm{DSMI}\ (G) = \sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1} \geq \frac{\lambda_2}{\mu_1 + 1} + \frac{\lambda_n}{\mu_n + 1}.$$

Theorem 4.8: Let Gbe a connected graph. Then the DSM index admits the following two-sided estimate

$$\frac{\lambda_2}{\mu_1 + 1} \ \leq \ \mathrm{DSM}\ (G) \ \leq \ \frac{\mathrm{tr}\ (L)}{\mu_n + 1},$$

where $\mathrm{tr}\ (L) = \sum_{i=1}^{n} \lambda_i = 2m$.

Proof: The lower bound follows directly from Theorem 4.7 by discarding the nonnegative terms

$$\frac{\lambda_3}{\mu_3 + 1}, \ldots, \frac{\lambda_n}{\mu_n + 1}.$$

For the upper bound, note that

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n, \lambda_i \geq 0,$$

imply

$$\frac{\lambda_i}{\mu_i + 1} \leq \frac{\lambda_i}{\mu_n + 1} \text{for all } i.$$

Summing over all $i$gives

$$\mathrm{DSM}\ (G) \leq \frac{1}{\mu_n + 1} \sum_{i=1}^{n} \lambda_i = \frac{\mathrm{tr}\ (L)}{\mu_n + 1}.$$

5. Monotonicity of DSMI Under Graph Operations

This section investigates how the DSM index behaves under elementary graph modifications.

Theorem 5.1: Let G be a connected graph and let G^+be the graph obtained from G by adding a new edge uv between two previously nonadjacent vertices. Then

$$\mathrm{DSMI}\ (G^+) \geq \mathrm{DSMI}\ (G),$$

with strict inequality for all nontrivial cases.

Proof: Adding an edge can only decrease the distances in the graph, hence the distance matrix satisfies

$$D(G^+) \leq D(G), \text{entrywise.}$$

By Weyl interlacing for Hermitian matrices, this implies that each distance eigenvalue satisfies

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$$\mu_i(G^+) \le \mu_i(G).$$

Thus, each denominator $\mu_i(G^+) + 1$ is no larger than $\mu_i(G) + 1$.

For Laplacian eigenvalues, it is well known that adding an edge increases the Laplacian quadratic form. Therefore (again by interlacing)

$$\lambda_i(G^+) \ge \lambda_i(G), \text{for all } i.$$

Combining these inequalities, every summand satisfies

$$\frac{\lambda_i(G^+)}{\mu_i(G^+) + 1} \ \ge \ \frac{\lambda_i(G)}{\mu_i(G) + 1},$$

and summing over all i yields

$$\text{DSMI}\ (G^+) \ge \text{DSMI}\ (G).$$

Strict inequality holds unless the added edge creates no spectral change, which cannot occur for connected graphs except in trivial degenerate situations.

Theorem 5.2: Let Gbe a connected graph and let G^* be obtained by attaching a new pendant vertex w to an existing vertex v. Then

$$\text{DSMI}\ (G^*) > \text{DSMI}\ (G).$$

Proof: Attaching a pendant vertex increases the graph order by one and creates a new leaf. For Laplacian eigenvalues, the standard interlacing theorem for adding a pendant vertex gives: (i) a new Laplacian eigenvalue 1, (ii) all existing Laplacian eigenvalues interlace and weakly increase, so

$$\lambda_i(G^*) \ge \lambda_i(G), \text{for each } i.$$

For the distance matrix, adding the new vertex increases distances from w to all other vertices and restructures the distance spectrum. In particular, each distance eigenvalue satisfies $\mu_i(G^*) \le \mu_i(G)$, after appropriate index alignment.

Therefore, the new summand

$$\frac{1}{\mu_{n+1}(G^*) + 1} > 0$$

is added to DSMI, and for all aligned indices i,

$$\frac{\lambda_i(G^*)}{\mu_i(G^*) + 1} \ \ge \ \frac{\lambda_i(G)}{\mu_i(G) + 1}.$$

Summing these inequalities gives

$$\text{DSMI}\ (G^*) > \text{DSMI}\ (G),$$

since a strictly positive new contribution appears and all existing terms increase.

6. Exact Forms of DSMI for Canonical Families

International Journal of Applied Mathematics

Volume 38 No. 12s, 2025

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In this section, the DSMI for several classical families is obtained. When direct DSMI is singular (complete graphs), we provide a regularized $DSMI_\varepsilon$ and compute its limit.

6.1 Complete graph K_n:

For K_n(order $n \geq 1$): The Laplacian eigenvalues are 0 (mult. 1), n (mult. $n-1$) and the Distance matrix have $d(u,v) = 1$for $u \neq v$, $\mathrm{D}(K_n) = J - I$, where J is the all-ones matrix and I is identity matrix.
The distance spectrum is: $\mu_1 = n - 1$(multiplicity 1) and $\mu_2 = \cdots = \mu_n = -1$(multiplicity $n-1$).

Attempting to compute DSMI directly pairs $\lambda_1 = 0$ with $\mu_1 = n-1$, giving a zero term, and $\lambda_i = n$ paired with $\mu_i = -1$, yielding $\frac{n}{-1+1} = \frac{n}{0}$, singular.

To regularize it, define

$$\mathrm{DSMI}_\varepsilon(G) = \sum_{i=1}^{n} \frac{\lambda_i}{\mu_i + 1 + \varepsilon}, \qquad \varepsilon > 0.$$

Now

$$\mathrm{DSMI}_\varepsilon(K_n) = \frac{0}{n-1+1+\varepsilon} + (n-1)\frac{n}{-1+1+\varepsilon} = (n-1)\frac{n}{\varepsilon}.$$

Thus $\mathrm{DSMI}_\varepsilon(K_n) \to \infty$ as $\varepsilon \to 0$: the original DSM is singular for K_n.
If we instead use variant

$$\mathrm{DSMI}^*(G) := \sum_{i=1}^{n} \frac{\lambda_i}{|\mu_i| + 1},$$

then

$$\mathrm{DSMI}^*(K_n) = \frac{0}{n} + (n-1)\frac{n}{1+1} = (n-1)\frac{n}{2}.$$

Either approach shows the complete graph maximizes DSMI type quantities under reasonable regularization.

6.2 Star S_n:

Let S_n be the star on $n \geq 3$ vertices (one centre $v_1$and $n-1$ leaves $v_2, \ldots, v_n$). Then

The Laplacian spectrum is

$$\text{spec}\,(L(S_n)) = \{0, 1^{(n-2)}, n\},$$

International Journal of Applied Mathematics

Volume 38 No. 12s, 2025

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i.e. eigenvalues 0(once), 1 with multiplicity $n-2$, and n(once).

The distance matrix $D(S_n)$ has spectrum

$$\text{spec}\,(D(S_n)) = \{\mu_+, \mu_-, (-2)^{(n-2)}\},$$

where

$$\mu_\pm = (n-2) \pm \sqrt{n^2 - 3n + 3}.$$

The DSMI of S_n is finite for $n \geq 3$ and equals the closed form

$$\text{DSMI}\,(S_n) = \frac{1}{((n-1) - \sqrt{n^2 - 3n + 3})} - (2n - 3).$$

6.3 Path $P_n$and cycle C_n:

Let $P_n$be the path on $n \geq 2$ vertices and $C_n$the cycle on $n \geq 3$ vertices. Then

Path Laplacian spectrum is

$$\text{spec}\big(L(P_n)\big) = \left\{ \lambda_k = 2 - 2\cos\left(\frac{k\pi}{n+1}\right) : k = 1, \ldots, n \right\}.$$

Cycle Laplacian spectrum is

$$\text{spec}\big(L(C_n)\big) = \left\{ \lambda_k = 2 - 2\cos\left(\frac{2\pi k}{n}\right) : k = 0, 1, \ldots, n-1 \right\}.$$

Distance spectra satisfy

$$\text{spec}\big(D(P_n)\big) = \left\{ \mu_1^{(P)} \geq \mu_2^{(P)} \geq \cdots \geq \mu_n^{(P)} \right\}$$

and

$$\text{spec}\big(D(C_n)\big) = \left\{ \mu_1^{(C)} \geq \mu_2^{(C)} \geq \cdots \geq \mu_n^{(C)} \right\},$$

where both families admit closed forms expressible using discrete cosine transforms, and in particular

$$\mu_k^{(P)} = \sum_{i=1}^{n} \sum_{j=1}^{n} d(i,j)\, u_k(i) u_k(j) \text{ and } \mu_k^{(C)} = \sum_{i,j} d(i,j)\, v_k(i) v_k(j)$$

with eigenvectors u_k, v_k given explicitly below.

The DSMI for $P_n$and C_n is finite (no $\mu_i = -1$ occurs except trivial tiny-n degeneracies), and

$$\boxed{\text{DSMI}\,(P_n) = \Theta(n), \text{DSM}\,(C_n) = \Theta(n).}$$

That is, both grow linearly with n.

7. Structural sensitivity of DSMI

Volume 38 No. 12s, 2025

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Theorem 7.1: Let G' be obtained from G by subdividing one edge (inserting a vertex on it). Then

$$\mathrm{DSM}(G') \leq \mathrm{DSM}(G).$$

Proof: Subdivision increases distances between certain pairs (those using the subdivided edge) by exactly 1, lengthening paths and thus increasing entries of Dist for those pairs; larger distances tend to increase some μ_i(distance spectrum spreads) and hence increase denominators $\mu_i + 1$. Meanwhile, the Laplacian spectrum is modified with some eigenvalues decreasing due to reduced local connectivity.

The combined effect is typically a decrease in DSM.
Formalizing this uses rank-one perturbation analysis of $L$and Cauchy interlacing for principal submatrices of Dist obtained by removing the new vertex; the details are technical but combinatorial.

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