Edge Moment of a Graph: Structural Descriptors, Polynomial Representations, and Correlation with Octane Properties

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Abstract

In this paper, we introduce a new topological index, the Edge Moment of Graph denoted by $M_E^{\omega}(G)$, defined as the summation of the product of the distance between each pair of edges $d(e_i, e_j)$ in a graph G and their corresponding weight-sum $[\omega(e_i)+\omega(e_j)]$. Mathematically, $M_E^{\omega}(G) = \sum_{\substack{\{e_i,e_j\}\in E(G) \\ e_i \neq e_j}} d(e_i, e_j)\,[\omega(e_i)+\omega(e_j)]$. Alternatively, the Edge Moment can be expressed as $M_E^{\omega}(G) = \sum_{e\in E(G)} \omega(e)\, D_E(e)$, where $D_E(e) = \sum_{\substack{f\in E(G) \\ f\neq e}} d(e, f)$. We have obtained the closed form of this index for different classes of graphs such as the Path, Cycle, Star, Complete, Complete-Bipartite and Wheel graphs. As a special case, the edge moment index has been studied for different weight functions.

To prove the relevance and correctness of this newly defined topological index, we established a relation between the edge moment index and some well-known topological indices such as edge-Wiener, Schultz, and Zagreb indices. To strengthen its usefulness and application, we extend the definition of the edge moment index to Hyper-Edge Moment (HEM). We also define the edge moment polynomial $EP(G, x)$ and edge moment branching deviation ΔM_E, which is obtained analytically using $M_E^1(P_n)$ (the edge moment of unit weight path graph) and $M_E^1(G)$ (the unit weight edge moment of any graph G).

As an application, $EP(G, x)$ provides a strong structural descriptor capable of distinguishing the 18 isomers of octane (C_8H_{18}) when they have identical Wiener indices, demonstrating discriminating power beyond the classical distance-based descriptors. A Pearson correlation of $r = 0.9452$ is observed between the boiling point (B_p) and M_E^{ω} of n-alkanes. Furthermore, a strong correlation (r) of 0.9483 is obtained between ΔM_E and the Research Octane Number (RON) of the 18 isomers of octane, indicating a strong relationship. Moreover, validation is performed using Leave-One-Out Cross-Validation (LOOCV), which is the statistically appropriate method when $n = 18$. The resulting Leave-One-Out adjusted R^2 (LOO R^2) between HEM and RON is 0.8865. Therefore, HEM exhibits a strong correlation with RON and provides a more stable measure for prediction compared to ΔM_E and other classical topological indices.