Topological Indices of a Graph

Lecture Note

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Degree of Vertex in Graph

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$.

The degree $\deg(v)$ of a vertex v in G is the number of vertices adjacent to v.

The set of all vertices which adjacent to v is called *open neighborhood of v* and denoted by $N(v)$.

We obtain that

$$\deg(v) = |N(v)|$$

ve-Degree of Vertex in Graph

The *closed neighborhood of v* is the set

$$N[v] = N(v) \cup \{v\}.$$

The ve-degree $\deg_{ve}(v)$ of a vertex v in a graph G is the number of different edges that incident to any vertex from the closed neighborhood of v.

Degree Based Topological Indices

First Zagreb Index

$$M_1(G) = \sum_{u \in V(G)} \deg(u)^2 = \sum_{uv \in E(G)} [\deg(u) + \deg(v)]$$

Second Zagreb Index

$$M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v)$$

Degree Based Topological Indices

First General Zagreb Index

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} \deg(u)^{\alpha} = \sum_{uv \in E(G)} [\deg(u)^{\alpha-1} + \deg(v)^{\alpha-1}]$$

Degree Based Topological Indices

First Zagreb Coindex

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [\deg(u) + \deg(v)]$$

Second Zagreb Coindex

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} \deg(u)\deg(v)$$

Degree Based Topological Indices

Forgotten Topological Index or F-index

$$F(G) = \sum_{u \in V(G)} \deg(u)^3 = \sum_{uv \in E(G)} [\deg(u)^2 + \deg(v)^2]$$

Degree Based Topological Indices

First ve-degree Zagreb Index

$$M_{ve_1}(G) = \sum_{uv \in E(G)} [deg_{ve}(u) + deg_{ve}(v)]$$

Second ve-degree Zagreb Index

$$M_{ve_2}(G) = \sum_{uv \in E(G)} deg_{ve}(u)\, deg_{ve}(v)$$

Degree Based Topological Indices

F-ve-degree Index

$$F_{ve}(G) = \sum_{u \in V(G)} deg_{ve}(u)^3 = \sum_{uv \in E(G)} [deg_{ve}(u)^2 + deg_{ve}(v)^2]$$

Degree Based Topological Indices

Reduced Second Zagreb index

$$RM_2(G) = \sum_{uv \in E(G)} [\deg(u) - 1][\deg(v) - 1]$$

It implies that $RM_2(G) = M_2(G) - M_1(G) + m$

Degree Based Topological Indices

Narumi-Katayama Index

$$NK(G) = \prod_{v \in V(G)} \deg(v)$$

First Multiplicative Zagreb Index

$$\Pi_1(G) = \prod_{v \in V(G)} \deg(v)^2 = \prod_{uv \in E(G)} (\deg(u) + \deg(v))$$

and we have $\Pi_1(G) = NK(G)^2$

Second Multiplicative Zagreb Index

$$\Pi_2(G) = \prod_{uv \in E(G)} \deg(u)\deg(v)$$

Degree Based Topological Indices

Randic Index or Connectivity Index or Branching Index or Product-Connectivity Index (1975)

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\deg(u)\deg(v)} = \sum_{uv \in E(G)} (\deg(u)\deg(v))^{-1}$$

and

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg(u)\deg(v)}} = \sum_{uv \in E(G)} (\deg(u)\deg(v))^{-\frac{1}{2}}$$

Degree Based Topological Indices

Reciprocal Randic Index

$$R(G) = \sum_{uv \in E(G)} \sqrt{\deg(u)\deg(v)}$$

Reduced Reciprocal Randic Index

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{[\deg(u) - 1][\deg(v) - 1]}$$

Degree Based Topological Indices

The General Randic Index

$$R_\alpha(G) = \sum_{uv \in E(G)} (\deg(u)\deg(v))^\alpha$$

for an arbitrary $\alpha \in \mathbb{R}$.

When $\alpha = -1$ or $\alpha = -\frac{1}{2}$, we have the original Randic Index.

When $\alpha = 1$, we have the Second Zagreb Index.

Degree Based Topological Indices

The General Product-Connectivity Coindex

$$\overline{R_\alpha}(G) = \sum_{uv \notin E(G)} (\deg(u)\deg(v))^\alpha$$

for an arbitrary $\alpha \in \mathbb{R}$.

Degree Based Topological Indices

Atom-Bond-Connectivity Index

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u)\deg(v)}}$$

Harmonic Index

$$H(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)}$$

Degree Based Topological Indices

Augmented Zagreb Index

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{\deg(u)\deg(v)}{\deg(u) + \deg(v) - 2} \right)^3$$

Geometric-Arithmetic Index or First Geometric-Arithmetic Index

$$GA(G) = \sum_{uv \in E(G)} \frac{\sqrt{\deg(u)\deg(v)}}{\frac{(\deg(u) + \deg(v))}{2}} = \sum_{uv \in E(G)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u) + \deg(v)}$$

Degree Based Topological Indices

Sum-Connectivity Index

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg(u) + \deg(v)}} = \sum_{uv \in E(G)} (\deg(u) + \deg(v))^{-\frac{1}{2}}$$

Degree Based Topological Indices

General Sum-Connectivity Index

$$SCI_\alpha(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v))^\alpha$$

where α is any real numbers.

General Sum-Connectivity Coindex

$$\overline{SCI_\alpha}(G) = \sum_{uv \notin E(G)} (\deg(u) + \deg(v))^\alpha$$

where α is any real numbers

Distance Based Topological Indices

For all unordered pairs of vertices in graph G.

Wiener Index

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

Wiener Polarity Index

$$W_P(G) = d(G,3)$$

The number of vertex pairs of G whose the distance is k is denoted by $d(G,k)$.

Distance Based Topological Indices

Terminal Wiener Index

$$TW(G) = \sum_{\{u,v\} \subseteq V_1(G)} d(u,v)$$

where $V_1(G) \subseteq V(G)$ is the set of vertices of G whose degree is equal to one (the so-called pendent vertices or leaves).

Distance Based Topological Indices

Hyper Wiener Index

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} [d(u,v) + d(u,v)^2]$$

Reciprocal Complementary Wiener Index

$$RCW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{diam(G) - 1 + d(u,v)}$$

Diameter of G is denoted by $diam(G)$ and is defined as the greatest distance between any two vertices in G.

Distance Based Topological Indices

Old Harary Index

$$H_{old}(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)^2}$$

Harary Index

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)}$$

Eccentricity Based Topological Indices

The eccentricity $e(v)$ of a vertex v is the maximum distance from v to any other vertex in G.

Total Eccentricity

$$\xi(G) = \sum_{v \in V(G)} e(v)$$

Eccentricity Based Topological Indices

First Zagreb Eccentricity Index

$$E_1(G) = \sum_{u \in V(G)} (e(u))^2$$

Second Zagreb Eccentricity Index

$$E_2(G) = \sum_{uv \in E(G)} \mathrm{e}(u)\,\mathrm{e}(v)$$

Eccentricity Based Topological Indices

Eccentric Connectivity Index

$$\xi^c(G) = \sum_{v \in V(G)} e(v)\deg(v)$$

Connective Eccentricity Index

$$C^{\xi}(G) = \sum_{v \in V(G)} \frac{\deg(v)}{e(v)}$$

Eccentricity Based Topological Indices

$D(v)$ is defined as the sum of all distances from v in G.

Eccentric Distance Sum Index

$$\xi^d(G) = \sum_{v \in V(G)} e(v) D(v)$$

or

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V(G)} [e(u) + e(v)] d(u,v)$$

Eccentricity Based Topological Indices

Adjacent Eccentric Distance Sum Index

$$\xi^{sv}(G) = \sum_{v \in V(G)} \frac{e(v)D(v)}{\deg(v)}$$

Distance Degree Based Topological Indices

Degree Distance Index or Schultz Index

$$DD(G) = \sum_{u \neq v} (\deg(u) + \deg(v)) d(u, v)$$

Gutman Index

$$\mathrm{Gut}(G) = \sum_{u \neq v} \deg(u) \deg(v) d(u, v)$$

Distance Degree Based Topological Indices

Additively Weighted Harary Index or Reciprocal Degree Distance Index

$$H_A(G) = \sum_{u \neq v} \frac{(\deg(u) + \deg(v))}{d(u,v)}$$

Multiplicatively Weighted Harary Index

$$H_M(G) = \sum_{u \neq v} \frac{\deg(u)\deg(v)}{d(u,v)}$$

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