

ChemGraphX: An Open-Source Web Tool for Computing Topological Indices and Entropy Measures

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1 Topological Indices

A graph G consists of a pair $(V(G), E(G))$, where $V(G)$ and $E(G)$ are known as the vertex and edge set of G . In chemical graph theory a molecular structure of a chemical compound is often represented as a graph. The atoms present in a molecule are the elements of vertex set and bonds are the elements of edge set. The total number of elements in $|V(G)|$ and $|E(G)|$ are known as size and order of a graph. The number of edges incident to a vertex v is called the degree of that vertex and it is denoted by d_v . The collection of neighbors of vertex v is defined as $N(v) = \{u \in V(G) : uv \in E(G)\}$ and $s_v = \sum_{u \in N(v)} d_u$ denotes the neighborhood degree sum of vertex v .

Let us define degree and neighborhood degree sum based edge partition as $d_{(p,q)} = |\{uv \in E(G) : d_u = p, d_v = q\}|$ and $s_{(p,q)} = |\{uv \in E(G) : s_u = p, s_v = q\}|$. The measures such as size, order, degree and neighborhood degree sum based edge partitions are provided in graph information option of ChemGraphX.

1.1 Degree-Based Indices

Degree-based topological indices are computed based on the degrees associated with the end vertices of each edge in a graph G . Generic expression to compute degree-based indices is given as:

$$TI(G) = \sum_{e \in E(G)} f(e) \quad (1)$$

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Here $TI(G)$ is the topological index and $f(e)$ represents the edge function associated with the index. Each topological index has its neighborhood degree sum version, to differentiate both the versions we modify Equation 1 as:

$$TI^\delta(G) = \sum_{e=uv \in E(G)} f(\delta_u, \delta_v)$$

Where $\delta \in \{d, s\}$, by replacing δ with d and s we can obtain degree and neighborhood degree sum-based topological indices. ChemGraphX provides 26 degree-based indices along with neighborhood degree sum versions, mathematical formula to compute these indices are given as follows.

1. $ABC^\delta(G) = \sum_{uv \in E(G)} \frac{\delta_u + \delta_v - 2}{\sqrt{\delta_u \delta_v}}$, (Atom Bond Connectivity)
2. $AZ^\delta(G) = \sum_{uv \in E(G)} \left(\frac{\delta_u \delta_v}{\delta_u + \delta_v - 2} \right)^3$, (Augmented Zagreb)
3. $BM^\delta(G) = \sum_{uv \in E(G)} \delta_u + \delta_v + \delta_u \delta_v$, (Bi-Zagreb)
4. $BMG^\delta(G) = \sum_{uv \in E(G)} \frac{\delta_u + \delta_v + \delta_u \delta_v}{\sqrt{\delta_u \delta_v}}$, (Bi-Zagreb Geometric)
5. $BMH^\delta(G) = \sum_{uv \in E(G)} \frac{(\delta_u + \delta_v + \delta_u \delta_v)(\delta_u + \delta_v)}{2}$, (Bi-Zagreb Harmonic)
6. $M_1^\delta(G) = \sum_{uv \in E(G)} \delta_u + \delta_v$, (First Zagreb)
7. $F^\delta(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)^2 - 2\delta_u \delta_v$, (Forgotten)
8. $GA^\delta(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}$, (Geometric Arithmetic)
9. $GBM^\delta(G) = \sum_{uv \in E(G)} \frac{\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v + \delta_u \delta_v}$, (Geometric Bi-Zagreb)
10. $GH^\delta(G) = \sum_{uv \in E(G)} \frac{\sqrt{\delta_u \delta_v (\delta_u + \delta_v)}}{2}$, (Geometric Harmonic)
11. $GTM^\delta(G) = \sum_{uv \in E(G)} \frac{\sqrt{\delta_u \delta_v}}{\delta_u^2 + \delta_v^2 + \delta_u \delta_v}$, (Geometric Tri-Zagreb)
12. $H^\delta(G) = \sum_{uv \in E(G)} \frac{2}{\delta_u + \delta_v}$, (Harmonic)

13. $HBM^\delta(G) = \sum_{uv \in E(G)} \frac{2}{(\delta_u + \delta_v + \delta_u \delta_v)(\delta_u + \delta_v)}$, (Harmonic Bi-Zagreb)
14. $HG^\delta(G) = \sum_{uv \in E(G)} \frac{2}{\sqrt{\delta_u \delta_v}(\delta_u + \delta_v)}$, (Harmonic Geometric)
15. $HTM^\delta(G) = \sum_{uv \in E(G)} \frac{2}{(\delta_u^2 + \delta_v^2 + \delta_u \delta_v)(\delta_u + \delta_v)}$, (Harmonic Tri-Zagreb)
16. $HM^\delta(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)^2$, (Hyper Zagreb)
17. $IRR^\delta(G) = \sum_{uv \in E(G)} |\delta_u - \delta_v|$, (Irregularity Measure)
18. $R^\delta(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_u \delta_v}}$, (Randić)
19. $M_2^\delta(G) = \sum_{uv \in E(G)} \delta_u \delta_v$, (Second Zagreb)
20. $\sigma^\delta(G) = \sum_{uv \in E(G)} (\delta_u - \delta_v)^2$, (Sigma)
21. $SO^\delta(G) = \sum_{uv \in E(G)} \sqrt{\delta_u^2 + \delta_v^2}$,
22. $SC^\delta(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_u + \delta_v}}$, (Sum Connectivity)
23. $SDD^\delta(G) = \sum_{uv \in E(G)} \frac{(\delta_u + \delta_v)^2 - 2\delta_u \delta_v}{\delta_u \delta_v}$, (Symmetric Division Degree)
24. $TM^\delta(G) = \sum_{uv \in E(G)} \delta_u^2 + \delta_v^2 + \delta_u \delta_v$, (Tri-Zagreb)
25. $TMG^\delta(G) = \sum_{uv \in E(G)} \frac{\delta_u^2 + \delta_v^2 + \delta_u \delta_v}{\sqrt{\delta_u \delta_v}}$, (Tri-Zagreb Geometric)
26. $TMH^\delta(G) = \sum_{uv \in E(G)} \frac{(\delta_u^2 + \delta_v^2 + \delta_u \delta_v)(\delta_u + \delta_v)}{2}$, (Tri-Zagreb Harmonic)

1.2 Distance-Based Indices

The distance between any two vertices in G is defined as the length of the shortest path between those pairs and it is denoted by $D(u, v)$, $u, v \in V(G)$. The distance between any two pairs of edges $e = ab$, $f = cd \in E(G)$ is defined as the minimum number of edges along a shortest (e, c) -path or a shortest (e, d) -path and denoted by $D(e, f)$. Similarly we define distance between a vertex and edge

as $D(v, e) = \min(D(v, a), D(v, b))$, where $v \in V(G)$ and $e = ab \in E(G)$. For $e = uv \in E(G)$, we present the following notions to define various distance-based indices.

$$n_u = |\{a \in V(G) : D(u, a) < D(v, a)\}|$$

$$m_u = |\{h \in E(G) : D(u, h) < D(v, h)\}|$$

Further, n_v and m_v can be analogously defined with respect to v . ChemGraphX provides 24 distance-based indices which are listed below:

$$1. W_v(G) = \sum_{\{u,v\} \subseteq V(G)} D(u, v), \text{ (Wiener)}$$

$$2. W_e(G) = \sum_{\{e,f\} \subseteq E(G)} D(e, f), \text{ (Edge Wiener)}$$

$$3. W_{ve}(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{e \in E(G)} D(u, e), \text{ (Vertex-edge Wiener)}$$

$$4. SZ_v(G) = \sum_{uv \in E(G)} n_u n_v, \text{ (Szeged)}$$

$$5. SZ_e(G) = \sum_{uv \in E(G)} m_u m_v, \text{ (Edge Szeged)}$$

$$6. SZ_{ve}(G) = \frac{1}{2} \sum_{uv \in E(G)} n_u m_v + n_v m_u, \text{ (Vertex-edge Szeged)}$$

$$7. SZ_t(G) = SZ_v(G) + SZ_e(G) + 2SZ_{ve}(G), \text{ (Total Szeged)}$$

$$8. w^+ SZ_v(G) = \sum_{uv \in E(G)} (d_u + d_v) n_u n_v, \text{ (Weighted}^+ \text{ Szeged)}$$

$$9. w^* SZ_v(G) = \sum_{uv \in E(G)} (d_u d_v) n_u n_v, \text{ (Weighted}^* \text{ Szeged)}$$

$$10. w^+ SZ_e(G) = \sum_{uv \in E(G)} (d_u + d_v) m_u m_v, \text{ (Weighted}^+ \text{ edge Szeged)}$$

$$11. w^* SZ_e(G) = \sum_{uv \in E(G)} (d_u d_v) m_u m_v, \text{ (Weighted}^* \text{ edge Szeged)}$$

$$12. PI_v(G) = \sum_{uv \in E(G)} n_u + n_v, \text{ (Vertex Padmakar-Ivan)}$$

$$13. PI_e(G) = \sum_{uv \in E(G)} m_u + m_v, \text{ (Edge Padmakar-Ivan)}$$

$$14. w^+ PI_v(G) = \sum_{uv \in E(G)} (d_u + d_v)(n_u + n_v), \text{ (Weighted}^+ \text{ vertex Padmakar-Ivan)}$$

15. $w^*PI_v(G) = \sum_{uv \in E(G)} (d_u d_v)(n_u + n_v)$, (Weighted* vertex Padmakar–Ivan)
16. $w^+PI_e(G) = \sum_{uv \in E(G)} (d_u + d_v)(m_u + m_v)$, (Weighted⁺ edge Padmakar–Ivan)
17. $w^*PI_e(G) = \sum_{uv \in E(G)} (d_u d_v)(m_u + m_v)$, (Weighted* edge Padmakar–Ivan)
18. $MO_v(G) = \sum_{uv \in E(G)} |n_u - n_v|$, (Mostar)
19. $MO_e(G) = \sum_{uv \in E(G)} |m_u - m_v|$, (Edge Mostar)
20. $MO_t(G) = \sum_{uv \in E(G)} |(n_u + m_u) - (n_v + m_v)|$, (Total Mostar)
21. $w^+MO_v(G) = \sum_{uv \in E(G)} (d_u + d_v)|n_u - n_v|$, (Weighted⁺ Mostar)
22. $w^*MO_v(G) = \sum_{uv \in E(G)} (d_u d_v)|n_u - n_v|$, (Weighted* Mostar)
23. $w^+MO_e(G) = \sum_{uv \in E(G)} (d_u + d_v)|m_u - m_v|$, (Weighted⁺ edge Mostar)
24. $w^*MO_e(G) = \sum_{uv \in E(G)} (d_u d_v)|m_u - m_v|$, (Weighted* edge Mostar)

ChemGrapX implements a comprehensive set of topological indices, comprising the 26 degree-based indices together with their corresponding neighborhood degree variants yielding a total of 52 indices, along with the 24 distance-based indices defined in this section. In total, the web tool is capable of computing 76 distinct topological indices.

2 Entropy Measures

Graph entropy was introduced as a tool to analyze the complexity of graphs. Though there exist many approaches to determine probabilistic entropy, we use a statistical model developed by Shannon, because of its potential applications in different sciences like physical dissipative structures, biological systems, engineering sectors and so on.

The expression to compute graph entropy is given as:

$$Ent_{TI}(G) = - \sum_{e \in E(G)} p_e \ln(p_e) \quad (2)$$

Here p_e is the probability function and it is defined as:

$$p_e = \frac{f(e)}{\sum_{e \in E(G)} f(e)} = \frac{f(e)}{TI(G)}$$

Further, Equation 2 can be simplified as:

$$Ent_{TI}(G) = \ln(TI(G)) - \frac{1}{\ln(TI(G))} \sum_{e \in E(G)} f(e) \ln(f(e)) \quad (3)$$

We induce degree and distance-based topological indices with Equation 3 to compute various entropies. ChemGraphX provides 73 entropy measures based on the defined topological indices except Wiener-type, because they are not defined with respect edge function.