

Fuzzy computational analysis of the backbone DNA network using fuzzy topological indices

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Abstract

Fuzzy topological indices have a significant impact and are gaining attention due to their multiple applications in various scientific domains and daily life fields. These indices have also been thoroughly investigated in fuzzy contexts or fuzzy graphs. A topological index is a single numerical parameter associated with the structure of graphs or networks that contains information to characterize the network's attributes as well as mathematical modelling. These indices have practical applications in a wide range of fields, including ecology, social networks, multi-criteria decision-making systems and neural networks. Due to these several applications topological indices are needed to define fuzzy graphs or networks. By modeling DNA molecular structure as a fuzzy graph where vertices represent atoms and edges are bonds with probabilistic membership values, we establish quantitative descriptors that capture the inherent uncertainties in bio-molecular interactions. We introduced the notation of several fuzzy topological indices, such as the first and second fuzzy Zagreb indices, the harmonic fuzzy Zagreb index and the randic fuzzy Zagreb index of the fuzzy backbone DNA network, in this work.

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1. Introduction

Fuzzy networks are a reliable model for investigating numerous natural motions, such as the movement of people between countries and the transit of data among internet routers, among other things [1]. Graphs or networks can be utilised in circumstances where things can be linked together using rules or relationships. Fuzzy graph theory is concerned with the uncertainty of vertices and edges referred to as membership values. There are many uncertainties or fuzziness in the real world. Because of fuzziness, researchers have devoted their efforts to investigating a new branch of mathematics known as "fuzzy graph" [2]. Traditional crisp graph representations sometimes rely on precise, deterministic interactions between nodes, which is rarely the case in biological systems. Uncertainty in DNA molecular interactions arises from experimental error and environmental changes. As a result, fuzzy graphs provide a more realistic framework by factoring uncertainty into vertex and edge definitions. Surprisingly, the membership values of the fuzzy graph differ from those of the crisp graph theory. Read the book [3] to learn the fundamentals of graph theory.

In recreational mathematics, fuzzy graphs are employed as an application tool. Fuzzy graphs have many applications in the actual world, including networking, communication, molecular structure of chemical compounds, airline operations, data mining, electrical network and genetic (DNA) research [2]. Deoxyribonucleic acid is the chemical that supplies all living creatures with the information necessary to read their genes. It is made up of two very long polynucleotide chains that are twisted around each other in a double helix formation [22]. Each of these chains is held together by a backbone consisting of deoxyribose, a sugar with five carbons that is coupled to phosphate groups and bases that contain nitrogen. The vertices of a molecular graph represent the atoms and the edges represent the bonds that hold the molecule together.

Several recent studies have applied fuzzy graph models to chemical and molecular structures. For instance, Mufti et al. [21, 23] investigated fuzzy Zagreb indices and Randic indices of pizza graphs and linear hydrocarbons, offering insight into degree-based topological properties under uncertainty. Similarly, Gong and Hua [20] developed fuzzy incidence graph models with new Wiener-type indices for analyzing molecular networks. However, unlike these models, our study focuses on the backbone DNA network, a biologically significant and structurally complex molecular system. By applying fuzzy topological indices to this structure, our work provides a more biologically grounded application and a novel contribution in interpreting structural properties of DNA under uncertainty, a perspective underexplored in previous research.

The entirety of the body's DNA is referred to as the "genome," and this is what the term "genome" refers to. One half of a person's DNA comes from their mother, while the other comes from their father. Together, these two halves make up a person's genetic makeup. Genes make up only one hundredth of one percent of the genome. Your body's ability to produce protein, as well as its quantity, timing and quality, are all under the control of the remaining 99 percent. Scientists continue to improve their understanding of how cells function when new biological problems are resolved and as new knowledge about the "non-coding" DNA backbone is discovered.

2. Preliminaries

A Fuzzy graph $\mathcal{FG} = (V, \sigma, \mu)$, V be the set of vertices together with two mappings $\sigma = V \rightarrow [0,1]$ and $\mu = V \times V \rightarrow [0,1]$. Such that, $\mu(u, v) \leq \min\{\sigma(u), \sigma(v)\}$, where, $u, v \in V$. Suppose $E(\mathcal{FG})$ be the set of edges. The only difference between a crisp graph and a fuzzy graph is the membership values assigned to the fuzzy graph's vertices and edges. If the membership values are equal and equal to one of all vertices and edges, the graph will be crisp [2]. Membership values are also known as vertices and edge weights, while vertices and edges with fuzzy weights are known as fuzzy vertex and fuzzy edges.

In a fuzzy graph [23], the degree of a vertex is calculated by adding the weights of all edges (which range from $[0,1]$) to the vertex (u), which is

$$d(u) = \sum \mu(uv).$$

The order $O(\mathcal{FG})$ and size $S(\mathcal{FG})$ of $\mathcal{FG}$ are obtained by adding the weights of all vertices and edges [23], i.e., $O(\mathcal{FG}) = \sum \sigma(u)$ and $S(\mathcal{FG}) = \sum \mu(uv)$.

Kalathian et al. [19] established the concept of fuzzy indices, which are defined as follows:

The first fuzzy Zagreb index $\mathcal{M}_1(\mathcal{FG})$ is defined as follows:

$$\mathcal{M}_1(\mathcal{FG}) = \sum_{r=1}^n \sigma(u_r) [d(u_r)]^2. \quad (1)$$

The second fuzzy Zagreb index $\mathcal{M}_2(\mathcal{FG})$ is defined as follows:

$$\mathcal{M}_2(\mathcal{FG}) = \frac{1}{2} \sum_{rs \in E(\mathcal{FG})} [\sigma(u_r)d(u_r)\sigma(v_s)d(v_s)]. \quad (2)$$

The fuzzy harmonic index $\mathcal{H}(\mathcal{FG})$ is defined as follows:

$$\mathcal{H}(\mathcal{FG}) = \frac{1}{2} \left[\sum_{rs \in E(\mathcal{FG})} \left[\frac{1}{\sigma(u_r)d(u_r) + \sigma(v_s)d(v_s)} \right] \right]. \quad (3)$$

The fuzzy Randic index $\mathcal{R}(\mathcal{FG})$ is defined as follows:

$$\mathcal{R}(\mathcal{FG}) = \frac{1}{2} \left[\sum_{r=1}^n \sigma(u_r)d(u_r)\sigma(v_s)d(v_s) \right]^{-1/2}. \quad (4)$$

The fuzzy graph of a backbone DNA network is the same as a crisp or simple backbone DNA network, the only difference is the membership values that are assigned to the vertices and edges. The vertices of this network represent atoms, while the edges represent bonds. Figure 1 depicts the backbone DNA network, while Figure 2 depicts the fuzzy graph of the backbone DNA network, denoted by $F(DNA_n)$. Vertex degrees (in red), vertex membership values (in black) and edge weights (in blue) reflect varying levels of certainty across the network's structure.

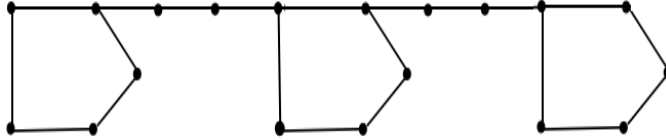


Figure 1
Backbone DNA Network.

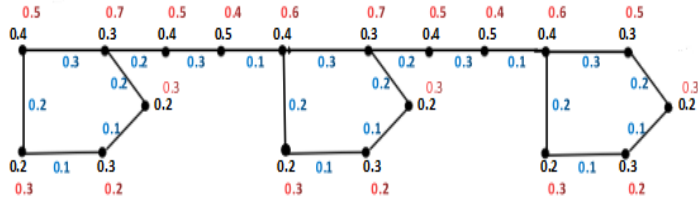


Figure 2
Fuzzy graph of Back bone DNA Network.

3. Literture Review

Zedah [4] introduced the concept of fuzziness. Rosenfeld first thought of fuzzy relations on fuzzy sets in 1975. Fuzzy graph theory was created by him. Bhattacharya [5] established the fuzzy analogues by utilising the fundamental result of graph theory, the characterization of the bridge in the fuzzy graph and also by introducing certain theoretical ideas of eccentricity and center. Palani, Kalavathi, and Mahalakshmi [6] introduced semi-fuzzy graphs and novel

definitions. Mordeson and Mathew [1] proposed an application of directed fuzzy networks in human trafficking and examined the notions of connection and dominance in directed fuzzy networks.

Many indices have been produced as a result of the application of topological indices in chemistry. The Wiener [7] index was the first topological index employed in chemistry. Topological indices play a significant role in modelling the molecular structure in chemical graph theory. Farahani [8] determined the first and second Zagreb indices, as well as the zagreb polynomials of $HAC_5C_6C_7$ nanotube. Huo et al. [9] investigated $TiO_2[m,n]$ Nanotubes. They calculated several degree-dependent topological indices for a $TiO_2[m,n]$ line graph. The harmonic index of a graph was introduced by Li and Shiu [10]. Kazemi [11] studied the multiplicative indices of molecular networks with tree structure, as well as the first and second multiplicative Zagreb indices. The Edge Mostar index of nano-structures and chemical structures was investigated by Imran, Akhter, and Iqbal [12]. For further information on topological indices, see [13-18, 24].

The fuzzy index is a topological index based on the fuzzy graph. Kalathian et al. [19] defined fuzzy graph topological indices and studied the applications and limitations of several fuzzy indices. Gong and Hua [20] created new Wiener and connection indices for bipolar fuzzy incidence graphs and acquired the properties of these indices by defining fuzzy membership functions. Mufti et al. [21] created fuzzy topological indices such as the first and second Zagreb indices, the Randic index and the harmonic index of the pizza graph. See [25-32] for further information on fuzzy graphs and indices.

4. Main Results

In this section, we compute the previously defined fuzzy topological indices (the first and second fuzzy zagreb index, the fuzzy harmonic index and the fuzzy randic index) for the fuzzy graph of the Backbone *DNA* network $F(DNA_n)$, where $n > 1$. Figure 2: Fuzzy graph representation of the backbone DNA network $F(DNA_3)$.

Table 1
Edge partition w.r.t to degree type.

Edge w. r. t Vertex Weight	Degree Type	Count
(0.3,0.4)	(0.7,0.5)	n
(0.3,0.2)	(0.7,0.3)	n-1
(0.3,0.2)	(0.5,0.3)	1
(0.3,0.2)	(0.2,0.3)	2n
(0.2,0.4)	(0.3,0.5)	1
(0.4,0.5)	(0.5,0.4)	n-1
(0.5,0.4)	(0.4,0.6)	n-1
(0.4,0.3)	(0.6,0.5)	1
(0.2,0.4)	(0.3,0.6)	n-1
(0.4,0.3)	(0.6,0.7)	n-2

Theorem 3.1: Let $\mathcal{F}(\text{DNA}_n)$ be a fuzzy graph of the backbone DNA network; then, the first fuzzy Zagreb index of the backbone DNA network is:

$$\mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] = [0.483n - 0.26].$$

Proof: In a fuzzy graph of backbone DNA network $\mathcal{F}(\text{DNA}_n)$, the number of vertices and edges is $7n - 2$ and $8n - 3$ where $n > 1$. The vertex set $V_{0.2}$ has a total vertices count $2n$, where the degree of these vertices is (0.3) . In vertex set $V_{0.3}$, the total vertices count $2n$ out of which n vertices are of degree (0.2) , $n-1$ vertices of degree (0.7) and 1 vertex of degree (0.5) . In vertex set $V_{0.4}$, the total vertices count $2n - 1$ out of which n vertices of degree (0.5) and $n-1$ vertices of degree (0.6) . In vertex set $V_{0.5}$, the total vertices count $n-1$, here $n-1$ vertices of degree (0.4) . As by using equation (1):

$$\mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] = \sum_{r=1}^n \sigma(u_r)[d(u_r)]^2.$$

$$\begin{aligned} \mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] &= (0.2)[2n(0.3)^2] + 0.3[n(0.2)^2 + (n-1)(0.7)^2 + (0.5)^2] \\ &\quad + 0.4[n(0.5)^2 + (n-1)(0.6)^2] + 0.5[(n-1)(0.4)^2]. \end{aligned}$$

$$\begin{aligned} \mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] &= 0.036 + 0.3[0.53n - 0.24] + 0.4[0.61n - 0.36] \\ &\quad + 0.5[0.16n - 0.16]. \end{aligned}$$

$$\mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] = [0.036 + 0.159n - 0.072 + 0.244n - 0.144 + 0.08n - 0.08].$$

$$\mathcal{M}_1[\mathcal{F}(\text{DNA}_n)] = [0.483n - 0.26].$$

Theorem 3.2: Let $\mathcal{F}(\text{DNA}_n)$ be a fuzzy graph of backbone DNA network; then, the second fuzzy Zagreb index of backbone DNA network is:

$$\mathcal{M}_2[\mathcal{F}(\text{DNA}_n)] = [0.1073n - 0.0794].$$

Proof: In fuzzy graph of backbone DNA network $\mathcal{F}(\text{DNA}_n)$, the number of vertices and edges is $7n - 2$ and $8n - 3$, where, $n > 1$. Using Table 1 and Equation (2):

$$\mathcal{M}_2[\mathcal{F}(\text{DNA}_n)] = \frac{1}{2} \sum_{rs \in E[\mathcal{F}(\text{DNA}_n)]} [\sigma(u_r)d(u_r)\sigma(v_s)d(v_s)].$$

$$\begin{aligned} \mathcal{M}_2[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2}[n][0.042] + \frac{1}{2}[n-1][0.0126] + \frac{1}{2}[0.009] \\ &\quad + \frac{1}{2}[2n][0.0036] + \frac{1}{2}[0.012] + \frac{1}{2}[n-1][0.04] \\ &\quad + \frac{1}{2}[n-1][0.048] + \frac{1}{2}[0.036] + \frac{1}{2}[n-1][0.0144] \\ &\quad + \frac{1}{2}[n-2][0.0504]. \end{aligned}$$

$$\begin{aligned} \mathcal{M}_2[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2}[[0.042n] + [0.0126n - 0.0126] + 0.009 + [0.0072n] \\ &\quad + 0.012 + [0.04n - 0.04] + [0.048n - 0.048] + 0.036 \\ &\quad + [0.0144n - 0.0144] + [0.0504n - 0.1008]]. \end{aligned}$$

$$\mathcal{M}_2[\mathcal{F}(\text{DNA}_n)] = [0.1073n - 0.0794].$$

Theorem 3.3: Let $\mathcal{F}(\text{DNA}_n)$ be a fuzzy graph of backbone DNA network; then, the harmonic fuzzy Zagreb index of backbone DNA network is:

$$\mathcal{H}[\mathcal{F}(\text{DNA}_n)] = [16.5687n + 2.5410].$$

Proof: In fuzzy graph of backbone DNA network $\mathcal{F}(\text{DNA}_n)$, the number of vertices and edges is $7n - 2$ and $8n - 3$, where $n > 1$, Using Table 1 and Equation (2):

$$\begin{aligned} \mathcal{H}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} \left[\sum_{rs \in E[\mathcal{F}(\text{DNA}_n)]} \left[\frac{1}{\sigma(u_r)d(u_r) + \sigma(v_s)d(v_s)} \right] \right] \\ \mathcal{H}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} \left[\frac{n}{(0.3)(0.7) + (0.4)(0.5)} \right] + \frac{1}{2} \left[\frac{n-1}{(0.3)(0.7) + (0.2)(0.3)} \right] + \frac{1}{2} \left[\frac{1}{(0.3)(0.5) + (0.2)(0.3)} \right] \\ &+ \frac{1}{2} \left[\frac{2n}{(0.3)(0.2) + (0.2)(0.3)} \right] + \frac{1}{2} \left[\frac{1}{(0.2)(0.3) + (0.4)(0.5)} \right] + \frac{1}{2} \left[\frac{n-1}{(0.4)(0.5) + (0.5)(0.4)} \right] + \frac{1}{2} \left[\frac{n-1}{(0.5)(0.4) + (0.4)(0.6)} \right] \\ &+ \frac{1}{2} \left[\frac{1}{(0.4)(0.6) + (0.3)(0.5)} \right] + \frac{1}{2} \left[\frac{n-1}{(0.2)(0.3) + (0.4)(0.6)} \right] + \frac{1}{2} \left[\frac{n-2}{(0.4)(0.6) + (0.3)(0.7)} \right]. \\ \mathcal{H}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} \left[\frac{n}{(0.41)} + \frac{n-1}{(0.27)} + \frac{1}{(0.21)} + \frac{2n}{(0.12)} + \frac{1}{(0.26)} + \frac{n-1}{(0.40)} + \frac{n-1}{(0.44)} + \frac{1}{(0.39)} + \frac{n-1}{(0.30)} + \frac{n-2}{(0.45)} \right]. \\ \mathcal{H}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} [2.4390n + 3.7037n - 3.7037 + 4.7619 + 16.6666n + 3.8461 + 2.5n - 2.5 \\ &+ 2.2727n - 2.2727 + 2.5641 + 3.3333n - 3.3333 + 2.2222n - 4.4444]. \\ \mathcal{H}[\mathcal{F}(\text{DNA}_n)] &= [16.5687n + 2.5410]. \end{aligned}$$

Theorem 3.4: Let $\mathcal{F}(\text{DNA}_n)$ be a fuzzy graph of backbone DNA network; then, the Randic fuzzy Zagreb index of backbone DNA network is:

$$\mathcal{R}[\mathcal{F}(\text{DNA}_n)] = [34.7360n - 5.3873].$$

Proof: In fuzzy graph of backbone DNA network $\mathcal{F}(\text{DNA}_n)$, the number of vertices and edges is $7n - 2$ and $8n - 3$ where $n > 1$, Using Table 1 and Equation (2):

$$\begin{aligned} \mathcal{R}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} \left[\sum_{r=1}^n \sigma(u_r)d(u_r)\sigma(v_s)d(v_s) \right]^{-1/2}. \\ \mathcal{R}[\mathcal{F}(\text{DNA}_n)] &= \frac{1}{2} [n][(0.3)(0.7)(0.4)(0.5)]^{-1/2} + \frac{1}{2} [n-1][(0.3)(0.7)(0.2)(0.3)]^{-1/2} \\ &+ \frac{1}{2} [(0.3)(0.5)(0.2)(0.3)]^{-1/2} + \frac{1}{2} [2n][(0.3)(0.2)(0.2)(0.3)]^{-1/2} \\ &+ \frac{1}{2} [(0.2)(0.3)(0.4)(0.5)]^{-1/2} + \frac{1}{2} [n-1][(0.4)(0.5)(0.5)(0.4)]^{-1/2} \\ &+ \frac{1}{2} [n-1][(0.5)(0.4)(0.4)(0.6)]^{-1/2} + \frac{1}{2} [(0.4)(0.6)(0.3)(0.5)]^{-1/2} \\ &+ \frac{1}{2} [n-1][(0.2)(0.3)(0.4)(0.6)]^{-1/2} + \frac{1}{2} [n-2][(0.4)(0.6)(0.3)(0.7)]^{-1/2}. \end{aligned}$$

$$\begin{aligned}
\mathcal{R}[\mathcal{F}(DNA_n)] &= \frac{1}{2}[n][0.042]^{-\frac{1}{2}} + \frac{1}{2}[n-1][0.0126]^{-\frac{1}{2}} + \frac{1}{2}[0.009]^{-\frac{1}{2}} \\
&+ \frac{1}{2}[2n][0.0036]^{-\frac{1}{2}} + \frac{1}{2}[0.012]^{-\frac{1}{2}} + \frac{1}{2}[n-1][0.04]^{-\frac{1}{2}} + \frac{1}{2}[n-1][0.048]^{-\frac{1}{2}} \\
&+ \frac{1}{2}[0.036]^{-\frac{1}{2}} + \frac{1}{2}[n-1][0.0144]^{-\frac{1}{2}} + \frac{1}{2}[n-2][0.0504]^{-\frac{1}{2}}. \\
\mathcal{R}[\mathcal{F}(DNA_n)] &= \frac{1}{2}[[4.8795n] + [8.9087n - 8.9087] + [10.5409] + [33.332n] \\
&+ [9.1287] + [5.0n - 5.0] + [4.5643n - 4.5643] + [5.2704] \\
&+ [8.3333n - 8.3333] + [4.4543n - 8.9086]]. \\
\mathcal{R}[\mathcal{F}(DNA_n)] &= [34.7360n - 5.3873].
\end{aligned}$$

Conclusion

This paper presents a novel use of fuzzy topological indices on DNA backbone structures. The indices obtained provide informative structural characterizations under uncertainty, which are useful in both theoretical and applied study. The importance of topological indices is increasing today. In a current research area, people are working with fuzzy topological indices. Numerous fuzzy topological indices introduced recently, few of them like first and second fuzzy zagreb index, harmonic fuzzy zagreb index and randic fuzzy zagreb index for backbone DNA network are calculate in this research work.

The values calculated for the Randic and fuzzy Zagreb indices give the DNA backbone network's structural fingerprints in the presence of noise or uncertainty. These measurements may show the probability of interactions within the genome or the stability of specific nucleotide configurations. Future research could examine the relationship between these fuzzy indices and experimental findings about the flexibility of DNA.

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