Research Article

On Topological Analysis of Niobium (II) Oxide Network via Curve Fitting and Entropy Measures

Muhammad Kamran Siddiqui, 1 Sana Javed, 1 Sadia Khalid, 1 Mazhar Hussain, 1 Muhammad Shahbaz, 1 and Samuel Asefa Fufa 2

1Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Pakistan
2Department of Mathematics, Addis Ababa University, Addis Ababa, Ethiopia

Correspondence should be addressed to Samuel Asefa Fufa; samuel.asefa@aau.edu.et

Received 24 April 2022; Revised 26 May 2022; Accepted 21 June 2022; Published 13 August 2022

Academic Editor: Yue Song

Copyright © 2022 Muhammad Kamran Siddiqui et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The remarkable optical features of metallic nanoparticles have extensively developed the interest of scientists and researchers. The generated heat overwhelms cancer tissue incident to nanoparticles with no damage to sound tissues. Niobium nanoparticles have the ability of easy ligands connection so they are very suitable in treating cancer optothermally. A modern field of applied chemistry is chemical graph theory. With the use of combinatorial methods, such as vertex and edge partitions, we explore the connection between atoms and bonds. Topological indices play a vital part in equipping directions to treat cancers or tumors. These indices might be derived experimentally or computed numerically. Although experimental results are worthwhile but they are expensive as well, so computational analysis provides an economical and rapid way. A topological index is a numerical value that is only determined by the graph. In this paper, we will discuss the chemical graph of niobium (II) oxide. Additionally, each topological index is related with thermodynamical properties of niobium (II) oxide, including entropy and enthalpy. This has been done in MATLAB software, using rational built-in method.

1. Introduction

All types of data quantitative, qualitative, processed, or unprocessed might be considered to gain information to address a simple or a complicated event or situation. If we consider the flow chart of the information, then on the top of the hierarchy we would find notion being the first qualitative obscure assessment of information. The central part of this flow chart comprises of the parameters and measurements while decision making extracted from inference is the final step. Different properties of a chemical compound like its nature, atoms, or chemical state provide us chemical information about the structure [1]. Different chemical reactions in a substance environment produce different physicochemical properties/activities that include boiling point, entropy, heat of formation, or density. In this way, the whole milieu of a substance becomes a promising root of information for the analysis of its chemistry [1]. Supplementary knowledge might be gained by in silico trials for the designing of new compounds for a specified study or objective. Stimulation in such approaches has been seen due to expensive experimental studies along with rigorous biotic and ecological regulations [2]. Such in silico studies are very progressive in medicine due to their cost effectiveness.

Different approaches including graphical quantitative/quantitative structure activity/property relationship (QSAR/QSPR) and modeling have become an essential part of in silico studies in drug development [3, 4]. This is due to the fact that biological variations can be explained in the form of chemical variations. Such analyses are performed continually to obtain profound results [5, 6]. Topological indices play a vital part in equipping directions to treat cancers or tumors. These indices might be derived experimentally or computed numerically [7, 8]. Although experimental results are worthwhile but they are expensive as well, so computational analysis provides an economical way Recently, several
studies are performed/reviewed using the concept of graph theoretical indices in drug research [9, 10]. There is a wide variety of such indices in the literature [11, 12].

A graph usually comprises of two sets, namely, vertex set, that contains the objects, and the edge set; this is based on the connections between the objects. Any chemical compound might be represented in the form of a graph where atoms make the vertex set and the bonding between atoms creates the edge set. Topological indices are based on the atomic connectivity table of the chemical compound [1]. Graphical descriptors, which are usually defined in the form of numerical numbers, can be used to appraise distinct immersed characteristics of a chemical compound from different point of view. Zagreb indices measure the compactness of a molecule so it can be correlated with the physicochemical properties of a compound which depend on the volume/surface ratio of the molecules.

The remarkable optical features of metallic nanoparticles have extensively developed the interest of scientists and researchers [13–15]. Researchers have analyzed that the thermoplasmonic features of nanoparticles might be utilized in treating cancers [16–18]. In optothermal cancer tissue therapy, the descendent laser light provokes the frequency of maximum response amplitude of external plasmon of metallic nanoparticles and consequently the immersed energy of descendent light preserves the heat in nanoparticles [19–21]. The generated heat overwhelms cancer tissue incident to nanoparticles with no damage to sound tissues [22, 23]. Niobium nanoparticles have the ability of easy ligands connection so they are very suitable in treating the cancer optothermally [24–26].

Niobium (Nb), a recalcitrant metal, is a suitable construction material for the first shell of nuclear fusion reactors [27]. It does, however, have a high affinity for oxygen and carbon, which are found in pyrotechnics and refrigerants such as liquid. Niobium is renowned to interact very efficiently with oxygen as a component for the first barrier. As a result, reliable thermodynamical data on niobium oxides, NbO, NbO2, Nb2O5, and other intermediary phases, such as Nb25O25, are useful. Apart from that, niobium oxides have a variety of innovative uses. Niobium monoxide (NbO) is utilized as a gate electrode in transistors [28], and a (NbO/NbO2) junction may be employed in robust switching devices [29]. NbO crystallises in the form of a face-centered cubic structure similar to sodium chloride crystal where every Nb atom in a square planar lattice is linked to four oxygen atoms [30]. Furthermore, the NbO crystal structure is unique in which it has 25 percent arranged voids in both the Nb and O sublattices as shown in Figure 1 [31].

Researchers have investigated the electrical and thermophysical properties of NbO. NbO has a density of around 7.3 g/cm³ and a melting temperature of 1940°C [31]. Niobium monoxide exhibits typical metallic behaviour and is usually recognized as a metal, with a resistivity of around 21 l × cm at 25°C that drops with temperature to 1.8 l × cm at 4.2 K. Researchers have measured X-ray fluorescence for several niobium oxides and correlated the findings of NbO to the conduction and valence band calculations of Nb1.0O0.33, discovering substantial variances [32]. They attempted to emulate the NbO structure by doing band structure calculations for Nb0.75O0.25 in order to account for the 25% vacancy (see Figure 1). However, the investigation pertaining to the thermodynamic data is very scarce. The laboratory work to study these characteristics is limited due to the analytical limitations. Therefore, computational techniques can be applied to estimate their thermodynamic characteristics. Topological study is useful in this regard [31].

Milan Randić presented the following index, namely, General Randić index [33–35] for a graph \( G = (V,E) \), where \( \mathcal{U}(a) \) denotes the degree of a vertex \( a \) as the number of edges with \( a \):

\[
R_a(G) = R_a = \sum_{lm \in E(G)} \left( \mathcal{U}(l) \times \mathcal{U}(m) \right)^{\alpha},
\]

where \( \alpha \in \{1, -1, \frac{1}{2}, -\frac{1}{2}\}, 2 \).

Estrada et al. [36, 37] established atom bond connectivity index as follows:

\[
ABC(G) = ABC = \sum_{lm \in E(G)} \sqrt{\mathcal{U}(l) + \mathcal{U}(m) - 2} \mathcal{U}(l) \times \mathcal{U}(m).
\]

Vukičević and Furtula [38] presented the geometric arithmetic index as follows:

\[
GA(G) = GA = \sum_{lm \in E(G)} 2\sqrt{\mathcal{U}(l) \times \mathcal{U}(m)} \mathcal{U}(l) + \mathcal{U}(m).
\]

The Zagreb indices defined in [20, 39, 40] are as follows:

\[
M_1(G) = M_1 = \sum_{lm \in E(G)} \mathcal{U}(l) \times \mathcal{U}(m),
\]

\[
M_2(G) = M_2 = \sum_{lm \in E(G)} \mathcal{U}(l) \times \mathcal{U}(m).
\]

The first and second Zagreb coindices defined in [41, 42] are as follows:

\[
\overline{M}_1(G) = \overline{M}_1 = \sum_{lm \notin E(G)} \mathcal{U}(l) \times \mathcal{U}(m),
\]

\[
\overline{M}_2(G) = \overline{M}_2 = \sum_{lm \notin E(G)} \mathcal{U}(l) \times \mathcal{U}(m).
\]
Gutman and Trinajstić [40] and Furtula and Gutman [43] introduced forgotten index as follows:

$$F(G) = F = \sum_{l \in V(G)} \left( \mathcal{Q}(l)^2 + \mathcal{Q}(m)^2 \right).$$  \hspace{1cm} (6)

Wang et al. [44] described the augmented Zagreb index as

$$\text{AZI}(G) = \text{AZI} = \sum_{l \in I_{E(G)}} \left( \frac{\mathcal{Q}(l) \times \mathcal{Q}(m)}{\mathcal{Q}(l) + \mathcal{Q}(m) - 2} \right)^3.$$  \hspace{1cm} (7)

The Balaban index [45, 46] is presented as follows:

$$J(G) = J = \frac{1}{l-m} \sum_{l \in I_{E(G)}} \frac{1}{\mathcal{Q}(l) \times \mathcal{Q}(m)}.$$  \hspace{1cm} (8)

Ranjini et al. in [47] reformulated versions of Zagreb indices as follows:

$$\text{ReZG}_1(G) = \text{ReZG}_1 = \sum_{l \in I_{E(G)}} \frac{\mathcal{Q}(l) + \mathcal{Q}(m)}{\mathcal{Q}(l) \times \mathcal{Q}(m)}.$$  \hspace{1cm} (9)

$$\text{ReZG}_2(G) = \text{ReZG}_2 = \sum_{l \in I_{E(G)}} \frac{\mathcal{Q}(l) \times \mathcal{Q}(m)}{\mathcal{Q}(l) + \mathcal{Q}(m)}.$$  \hspace{1cm} (9)

$$\text{ReZG}_3(G) = \text{ReZG}_3 = \sum_{l \in I_{E(G)}} (\mathcal{Q}(l) \times \mathcal{Q}(m))(\mathcal{Q}(l) + \mathcal{Q}(m)).$$

### 2. Results for Niobium (II) Oxide

The number of vertices and edges of structure of Niobium (II) oxide denoted by NbO is $9lm + 5l + 5m + 2$ and $16lm + 6l + 6m$, respectively. In NbO there are three types of vertices, namely, the vertices of degree 2, 3, and 4, respectively. The vertex and edge partition of NbO is presented in Table 1 and Table 2, respectively.

**Theorem 1.** Let $G \cong \text{NbO}[l, m]$ with $l, m \geq 1$. Then, Randić indices for $\alpha \in \{1, -1, 1/2, -1/2\}$ are as follows:

$$R_1 = 208lm + 16l + 16m - 24,$$

$$R_{-1} = 1.125lm + 1.1111l + 0.9861m + 0.6666,$$

$$R_{1/2} = 49.5692lm + 20.2871l + 12.2871m - 5.0953,$$

$$R_{-1/2} = 3.964lm + 3.0239l + 2.5239m + 0.8413.$$  \hspace{1cm} (10)

**Proof.** For $\alpha = 1$,

$$R_1 = \sum_{l \in I_{E(G)}} \mathcal{Q}(l) \times \mathcal{Q}(m)$$

$$= (16)(6) + (16l + 16m - 24)(9)$$

$$+ (12lm - 8l - 8m + 8)(12) + (4lm - 2l - 2m)(16)$$

$$= 208lm + 16l + 16m - 24.$$  \hspace{1cm} (11)

<table>
<thead>
<tr>
<th>Table 1: Vertex partition of NbO.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathcal{Q}(v) )</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2: Edge partition of NbO.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathcal{Q}(l), \mathcal{Q}(m) )</td>
</tr>
<tr>
<td>(2, 3)</td>
</tr>
<tr>
<td>(3, 3)</td>
</tr>
<tr>
<td>(3, 4)</td>
</tr>
<tr>
<td>(4, 4)</td>
</tr>
</tbody>
</table>

For $\alpha = -1$,

$$R_{-1} = \sum_{l \in I_{E(G)}} \frac{1}{\mathcal{Q}(l) \times \mathcal{Q}(m)}$$

$$= (16)\left(\frac{1}{6}\right) + (16l + 16m - 24)\left(\frac{1}{9}\right)$$

$$+ (12lm - 8l - 8m + 8)\left(\frac{1}{12}\right)$$

$$+ (4lm - 2l - 2m)\left(\frac{1}{16}\right)$$

$$= 1.125lm + 1.1111l + 0.9861m + 0.6666.$$  \hspace{1cm} (12)

For $\alpha = 1/2$,

$$R_{1/2} = \sum_{l \in I_{E(G)}} \sqrt{\mathcal{Q}(l) \times \mathcal{Q}(m)}$$

$$= (16)\left(\frac{1}{\sqrt{6}}\right) + (16l + 16m - 24)\left(\frac{1}{\sqrt{9}}\right)$$

$$+ (12lm - 8l - 8m + 8)\left(\frac{1}{\sqrt{12}}\right)$$

$$+ (4lm - 2l - 2m)\left(\frac{1}{\sqrt{16}}\right)$$

$$= 49.5692lm + 20.2871l + 12.2871m - 5.0953.$$  \hspace{1cm} (13)

For $\alpha = -1/2$,

$$R_{-1/2} = \sum_{l \in I_{E(G)}} \frac{1}{\sqrt{\mathcal{Q}(l) \times \mathcal{Q}(m)}}$$

$$= (16)\left(\frac{1}{\sqrt{6}}\right) + (16l + 16m - 24)\left(\frac{1}{\sqrt{9}}\right)$$

$$+ (12lm - 8l - 8m + 8)\left(\frac{1}{\sqrt{12}}\right)$$

$$+ (4lm - 2l - 2m)\left(\frac{1}{\sqrt{16}}\right)$$

$$= 3.964lm + 3.0239l + 2.5239m + 0.8413.$$  \hspace{1cm} (14)
Theorem 2. Let $G \equiv \text{NbO}$, with $l,m \geq 1$. Then, the atom bond connectivity index corresponds to

$$ABC = 10.1954lm + 4.2779l + 4.2779m + 0.4776. \quad (15)$$

Proof

$$ABC = \sum_{l,m \in E(G)} \left( \frac{\mathcal{Q}(l) + \mathcal{Q}(m) - 2}{\mathcal{Q}(l) \times \mathcal{Q}(m)} \right)$$

$$= (16) \left( \frac{3}{5} \right) + (16l + 16m - 24) \left( \frac{4}{9} \right)$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{5}{12} \right)$$

$$+ (4lm - 2l - 2m) \left( \frac{6}{16} \right)$$

$$= 10.1954lm + 4.2779l + 4.2779m + 0.4776. \quad \square$$

Theorem 3. Consider the graph of $G \equiv \text{NbO}$ which has $l,m \geq 1$ and geometric arithmetic index is corresponding to the following:

$$GA = 15.8769lm + 6.0820l + 6.0820m - 0.4053. \quad (17)$$

Proof

$$GA = \sum_{l,m \in E(G)} \frac{2 \sqrt{\mathcal{Q}(l) \times \mathcal{Q}(m)}}{\mathcal{Q}(l) + \mathcal{Q}(m)}$$

$$= (16) \left( \frac{2 \sqrt{6}}{5} \right) + (16l + 16m - 24) \left( \frac{2 \sqrt{5}}{6} \right)$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{2 \sqrt{12}}{7} \right)$$

$$+ (4lm - 2l - 2m) \left( \frac{2 \sqrt{16}}{8} \right)$$

$$= 15.8769lm + 6.0820l + 6.0820m - 0.4053. \quad \square$$

Theorem 4. The forgotten index for the graph of $G \equiv \text{NbO}[l,m]$ with $l,m \geq 1$ is corresponding to

$$F = 428lm + 24l + 24m - 24. \quad (19)$$

Proof

$$F = \sum_{l,m \in E(G)} \left( \frac{\mathcal{Q}(l)^2 + \mathcal{Q}(m)^2}{\mathcal{Q}(l) + \mathcal{Q}(m)} \right)$$

$$= (16) \left( \frac{15}{6} \right) + (16l + 16m - 24) \left( \frac{12}{7} \right)$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{16}{17} \right)$$

$$+ (4lm - 2l - 2m) \left( \frac{16}{17} \right)$$

$$= 428lm + 24l + 24m - 24. \quad \square$$

Theorem 5. The augmented index for the graph of $G \equiv \text{NbO}[l,m]$ with $l,m \geq 1$ is corresponding to

$$AZI = 241.7398lm + 33.7320l + 33.7320m - 34.783. \quad (21)$$

Proof

$$AZI = \sum_{l,m \in E(G)} \left( \frac{\mathcal{Q}(l) \times \mathcal{Q}(m)}{\mathcal{Q}(l) + \mathcal{Q}(m) - 2} \right)^3$$

$$= (16) \left( \frac{6}{3} \right)^3 + (16l + 16m - 24) \left( \frac{9}{4} \right)^3$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{12}{5} \right)^3$$

$$+ (4lm - 2l - 2m) \left( \frac{16}{6} \right)^3$$

$$= 241.7398lm + 33.7320l + 33.7320m - 34.783. \quad \square$$

Theorem 6. Consider the graph of $G \equiv \text{NbO}[l,m]$ such that $l,m \geq 1$ and the first and second Zagreb index is corresponding to

$$M_1 = 116lm + 24l + 24m - 8,$$

$$M_2 = 208lm + 16l + 16m - 24. \quad (23)$$

Proof

$$M_1 = \sum_{l,m \in E(G)} \mathcal{Q}(l) + \mathcal{Q}(m)$$

$$= (16) \left( 5 + (16l + 16m - 24) \right) \left( \frac{6}{5} \right)$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{7}{6} \right)$$

$$+ (4lm - 2l - 2m) \left( \frac{8}{17} \right)$$

$$= 116lm + 24l + 24m - 8,$$

$$M_2 = \sum_{l,m \in E(G)} \mathcal{Q}(l) \times \mathcal{Q}(m)$$

$$= (16) \left( 6 + (16l + 16m - 24) \right) \left( \frac{9}{4} \right)$$

$$+ (12lm - 8l - 8m + 8) \left( \frac{12}{5} \right)$$

$$+ (4lm - 2l - 2m) \left( \frac{16}{6} \right)$$

$$= 208lm + 16l + 16m - 24. \quad \square$$

Complexity
Figure 2: Continued.
Figure 2: An interactive view of scattered plot together with surface plot of indices. (a) \((m, n, R_1)\). (b) \((m, n, R_{-1})\). (c) \((m, n, R_{1/2})\). (d) \((m, n, R_{-1/2})\). (e) \((m, n, \text{ABC})\). (f) \((m, n, \text{GA})\). (g) \((m, n, F)\). (h) \((m, n, \text{AZI})\). (i) \((m, n, M_1)\). (j) \((m, n, M_2)\). (k) \((m, n, \overline{M_1})\). (l) \((m, n, \overline{M_2})\). (m) \((m, n, \text{ReZG}_1)\). (n) \((m, n, \text{ReZG}_2)\). (o) \((m, n, \text{ReZG}_3)\).
The first and second Zagreb coindices for the graph of \( G \equiv \text{NbO}[l, m] \) with \( l, m \geq 1 \) are corresponding to

\[
\begin{align*}
\mathcal{M}_1 &= 288l^2m^2 + 268l^2m + 268lm^2 + 60l^2 \\
&\quad + 36lm + 60m^2 - 12l - 12m + 8, \\
\mathcal{M}_2 &= 512l^2m^2 + 384l^2m + 384lm^2 + 72l^2 \\
&\quad - 122lm + 72m^2 - 28l - 28m + 28.
\end{align*}
\]

(25)

Proof

\[
\mathcal{M}_1 = \sum_{lm \notin E(G)} \mathcal{Q}(l) + \mathcal{Q}(m) \\
= 2|E(G)|(|V(G)| - 1) - M_1 \\
= 2(16lm + 6l + 6m)(9lm + 5l + 5m + 2 - 1) \\
- (116lm + 24l + 24m - 8) \\
= 288l^2m^2 + 268l^2m + 268lm^2 + 60l^2 \\
+ 36lm + 60m^2 - 12l - 12m + 8,
\]

(26)

\[
\mathcal{M}_2 = \sum_{lm \notin E(G)} \mathcal{Q}(l) \times \mathcal{Q}(m) \\
= 2|E(G)|^2 - \frac{1}{2}M_1 - M_2 \\
= 2(16lm + 6l + 6m)^2 \\
- \frac{1}{2}(116lm + 24l + 24m - 8) \\
- (208lm + 16l + 16m - 24) \\
= 512l^2m^2 + 384l^2m + 384lm^2 \\
+ 72l^2 - 122lm + 72m^2 - 28l - 28m + 28.
\]

\( \Box \)

Theorem 8. The redefined Zagreb indices for the graph of \( G \equiv \text{NbO}[l, m] \) with \( l, m \geq 1 \) correspond to

\[
\begin{align*}
\text{ReZG}_1 &= 9lm + 5l + 5m + 2, \\
\text{ReZG}_2 &= 28.5714lm + 6.2857l + 6.2857m - 3.0857, \\
\text{ReZG}_3 &= 1520lm - 64l - 64m - 144.
\end{align*}
\]

(27)

Proof

\[
\text{ReZG}_1 = \sum_{lm \notin E(G)} \mathcal{Q}(l) + \mathcal{Q}(m) \\
= (16\left(\frac{6}{5}\right) + 16l + 16m - 24)\left(\frac{6}{9}\right) \\
+ (12lm - 8l - 8m + 8)\left(\frac{7}{12}\right) \\
+ (4lm - 2l - 2m)\left(\frac{8}{16}\right) \\
= 9lm + 5l + 5m + 2,
\]

(28)

\[
\text{ReZG}_2 = \sum_{lm \notin E(G)} \mathcal{Q}(l) \times \mathcal{Q}(m) \\
= (16\left(\frac{6}{5}\right) + 16l + 16m - 24)\left(\frac{9}{6}\right) \\
+ (12lm - 8l - 8m + 8)\left(\frac{12}{7}\right) \\
+ (4lm - 2l - 2m)\left(\frac{16}{8}\right) \\
= 28.5714lm + 6.2857l + 6.2857m - 3.0857,
\]

\[
\text{ReZG}_3 = \sum_{lm \notin E(G)} (\mathcal{Q}(l) \times \mathcal{Q}(m))(\mathcal{Q}(l) + \mathcal{Q}(m)) \\
= (16)(30) + (16l + 16m - 24)(54) \\
+ (12lm - 8l - 8m + 8)(84) \\
+ (4lm - 2l - 2m)(128) \\
= 1520lm - 64l - 64m - 144.
\]
Graphical illustration for each index corresponding to $l = m = i; i = 1, 2, \ldots, 100$, computed above, is provided in Figure 2.

2.1. Thermodynamical Properties (HoF and Entropy) of Niobium (II) Oxide. Many topological indices are derived for unit cell of NbO, including $M_1^i; M_1; ABC; GA$; and AZI.
These indices are linked to thermodynamic properties of NbO, such as heat of formation (HoF) or enthalpy and entropy. The standard molar enthalpy and entropy of NbO is $-405.8 \text{ kJ mol}^{-1}$ and $48.1 \text{ J mol}^{-1} \text{ K}^{-1}$, respectively. Table 3 represents the numerical values of HoF and Entropy.

2.2. Statistical Models for HoF and Topological Indices. In this section, mathematical frameworks are created for the topological index (computed in Section 2) and HoF (given in Section 2.1) of NbO. All fitted curves are shown in Figures 3–17 and also the constant quantity values of the
fitted curves are depicted in Tables 4–18. Also, the goodness of fit for indices vs. HoF for NbO is depicted in Table 19. Let \( \varepsilon \) and \( c \) denote the mean and standard deviation that is used to rescale the data.

(i) Estimation of rational polynomial for HoF vs. \( R_1 \) is

\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^4 + q_1 x^3 + q_2 x^2 + q_3 x + q_4},
\]  

where \( x = R_1 \) is rescaled through \( \varepsilon = 4264 \) and \( \gamma = 3746 \).
(ii) Estimation of rational polynomial for HoF vs. $R_{-1}$ is
\[
\text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^2 + q_1 x + q_2},
\]  
where $x = R_{-1}$ is rescaled through $\epsilon = 31.56$ and $\gamma = 24.34$.

(iii) Estimation of rational polynomial for HoF vs. $R_{1/2}$ is
\[
\text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},
\]  
where $x = R_{(1/2)}$ is rescaled through $\epsilon = 1117$ and $\gamma = 945.4$.

(iv) Estimation of rational polynomial for HoF vs. $R_{(-1/2)}$ is
\[
\text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^2 + q_1 x + q_2},
\]  
where $x = R_{(-1/2)}$ is rescaled through $\epsilon = 102.3$ and $\gamma = 81.85$.

(v) Estimation of rational polynomial for HoF vs. ABC is
\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^2 + q_1 x + q_2},
\]  
where $x = \text{ABC}$ is rescaled through $\epsilon = 238.6$ and $\gamma = 198.4$.

(vi) Estimation of rational polynomial for HoF vs. GA is
\[
\text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x + q_1},
\]  
where $x = \text{GA}$ is rescaled through $\epsilon = 365.8$ and $\gamma = 306.5$.

(vii) Estimation of rational polynomial for HoF vs. $M_1$ is
\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^4 + q_1 x^3 + q_2 x^2 + q_3 x + q_4},
\]  
where $x = M_1$ is rescaled through $\epsilon = 2504$ and $\gamma = 2153$.

(viii) Estimation of rational polynomial for HoF vs. $M_2$ is
\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^3 + q_1 x^2 + q_2 x + q_3},
\]  
where $x = M_2$ is rescaled through $\epsilon = 4264$ and $\gamma = 3746$.

(ix) Estimation of rational polynomial for HoF vs. $M_1$ is
\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^2 + q_1 x + q_2},
\]  
where $x = M_1$ is rescaled through $\epsilon = 2504$ and $\gamma = 2153$.

(x) Estimation of rational polynomial for HoF vs. $M_2$ is
\[
\text{HoF}(x) = \frac{p_1 x + p_2}{x^3 + q_1 x^2 + q_2 x + q_3},
\]  
where $x = M_2$ is rescaled through $\epsilon = 4264$ and $\gamma = 3746$.

(xi) Estimation of rational polynomial for HoF vs. $F$ is
\[
\text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x + q_1},
\]  
where $x = F$ is rescaled through $\epsilon = 1818$ and $\gamma = 1625$.
\[ \text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x + q_1}, \quad (40) \]

where \( x = F \) is rescaled through \( \epsilon = 8728 \) and \( \gamma = 7669 \).

(viii) Estimation of rational polynomial for HoF vs. ReZG is

\[ \text{HoF}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^2 + q_1 x^2 + q_2 x + q_3}, \quad (41) \]

where \( x = \text{ReZG}_1 \) is rescaled through \( \epsilon = 222 \) and \( \gamma = 180.3 \).

(ix) Estimation of rational polynomial for HoF vs. ReZG is
\[
\text{HoF}(x) = - \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3}, \quad (42)
\]

where \( x = \text{ReZG}_2 \) is rescaled through \( \varepsilon = 618.6 \) and \( \gamma = 531.8 \).

(x) Estimation of rational polynomial for HoF vs. ReZG\( _3 \) is

\[
\text{HoF}(x) = - \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x + q_2}, \quad (43)
\]
where \( x = \text{ReZG}_3 \) is rescaled through \( \epsilon = 2.974e + 04 \) and \( y = 2.661e + 04 \).

2.3. Statistical Models for Entropy and Topological Indices.
In this section, mathematical frameworks for the topological index (computed in Section 2) and Entropy (given in Section 2.1) of NbO are shown. All fitted curves are shown in Figures 18–32, and the parametric values of the fitted curves are given in Tables 20–34. Also, the goodness of fit for indices vs. entropy for NbO is depicted in Table 35.

(i) Estimated rational polynomial of Entropy vs. \( R_1 \) is

\[
\text{Entropy}(x) = \frac{p_1 x + p_2}{x^3 + q_1 x^2 + q_2 x + q_3}
\]

where \( x = R_1 \) is rescaled through \( \epsilon = 4264 \) and \( y = 3746 \).

(ii) Estimated rational polynomial of Entropy vs. \( R_{-1} \) is

\[
\text{Entropy}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3}
\]

where \( x = R_{-1} \) is rescaled through \( \epsilon = 31.56 \) and \( y = 24.34 \).

(iii) Estimated rational polynomial of Entropy vs. \( R_{4/2} \) is

| Table 6: \( R_{4/2} \) vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | 3.108e + 07 | (−6.357e + 10, 6.364e + 10) | 229.4 | (−4.749e + 05, 4.753e + 05) |
| \( i = 2 \) | 8.362e + 07 | (−1.71e + 11, 1.711e + 11) | −6.361e + 04 | (−1.302e + 08, 1.301e + 08) |
| \( i = 3 \) | 5.528e + 07 | (−1.13e + 11, 1.131e + 11) | −1.04e + 05 | (−2.128e + 08, 2.126e + 08) |

| Table 7: \( R_{-1/2} \) vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | −3.55e + 07 | (−9.978e + 10, 9.971e + 10) | 6.963e + 04 | (−1.956e + 08, 1.957e + 08) |
| \( i = 2 \) | −9.948e + 07 | (−2.796e + 11, 2.794e + 11) | 1.305e + 05 | (−3.666e + 08, 3.668e + 08) |
| \( i = 3 \) | −6.838e + 07 | (−1.921e + 11, 1.92e + 11) | — | — |

| Table 8: ABC vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | −3.504e + 04 | (−6.796e + 04, −2111) | −3.75 | (−5.523, −1.977) |
| \( i = 2 \) | −4.081e + 04 | (−7.88e + 04, −2822) | 77.34 | (5.61, 149.1) |

| Table 9: GA vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | 4.637e + 05 | (−2.16e + 10, 2.16e + 10) | −4.433e + 04 | (−2.063e + 09, 2.063e + 09) |
| \( i = 2 \) | 2.091e + 07 | (−9.735e + 11, 9.736e + 11) | — | — |
| \( i = 3 \) | 2.35e + 07 | (−1.094e + 12, 1.094e + 12) | — | — |

| Table 10: \( M_1 \) vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | −8.239e + 04 | (−5.395e + 05, 3.747e + 05) | −3.054 | (−8.908, 2.8) |
| \( i = 2 \) | −9.506e + 04 | (−6.215e + 05, 4.314e + 05) | 3.673 | (−15.16, 22.51) |
| \( i = 3 \) | — | — | −4.831 | (−34.56, 24.9) |
| \( i = 4 \) | — | — | 177.9 | (−807.8, 1164) |

| Table 6: \( R_{4/2} \) vs. HoF. |
|---|---|---|---|
| \( p_i \) | CI | \( q_i \) | CI |
| \( i = 1 \) | 3.108e + 07 | (−6.357e + 10, 6.364e + 10) | 229.4 | (−4.749e + 05, 4.753e + 05) |
| \( i = 2 \) | 8.362e + 07 | (−1.71e + 11, 1.711e + 11) | −6.361e + 04 | (−1.302e + 08, 1.301e + 08) |
| \( i = 3 \) | 5.528e + 07 | (−1.13e + 11, 1.131e + 11) | −1.04e + 05 | (−2.128e + 08, 2.126e + 08) |
### Table 11: $M_2$ vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$-7.613e + 07$</td>
<td>($-9.059e + 10, 9.044e + 10$)</td>
<td>$442.4$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$-8.664e + 07$</td>
<td>($-1.031e + 11, 1.029e + 11$)</td>
<td>$-1634$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$-3.103e + 07$</td>
<td>($-5.683e + 07, -1.069$)</td>
<td>$1.614e + 05$</td>
</tr>
</tbody>
</table>

### Table 12: $M_1$ vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$-3053$</td>
<td>($-4237, -1869$)</td>
<td>$6.184$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$-6405$</td>
<td>($-1.054e+04, -2.273$)</td>
<td>$4.651$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$-3146$</td>
<td>($-5686, -606.9$)</td>
<td>$-6.947e+04$</td>
</tr>
</tbody>
</table>

### Table 13: $M_2$ vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$1.765e + 07$</td>
<td>($-2.879e + 12, 2.879e + 12$)</td>
<td>$-7.947e + 04$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$1.026e + 08$</td>
<td>($-1.673e + 13, 1.673e + 13$)</td>
<td>$-1.008e + 05$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$7.063e + 07$</td>
<td>($-1.152e + 13, 1.152e + 13$)</td>
<td>$-7.947e + 04$</td>
</tr>
</tbody>
</table>

### Table 14: AZI vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$-8568$</td>
<td>($-1.056e + 08, 1.056e + 08$)</td>
<td>$-1.092e + 04$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$5.206e + 06$</td>
<td>($-6.799e + 10, 6.8e + 10$)</td>
<td>$-1.092e + 04$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$5.894e + 06$</td>
<td>($-7.693e + 10, 7.694e + 10$)</td>
<td>$-1.092e + 04$</td>
</tr>
</tbody>
</table>

### Table 15: $F$ vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$2.344e + 04$</td>
<td>($-4.068e + 08, 4.069e + 08$)</td>
<td>$-1.46e + 04$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$6.948e + 06$</td>
<td>($-1.182e + 11, 1.182e + 11$)</td>
<td>$-1.46e + 04$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$7.852e + 06$</td>
<td>($-1.336e + 11, 1.336e + 11$)</td>
<td>$-1.46e + 04$</td>
</tr>
</tbody>
</table>

### Table 16: ReZG vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$4.092e + 07$</td>
<td>($-4.611e + 11, 4.611e + 11$)</td>
<td>$1129$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$1.012e + 08$</td>
<td>($-1.14e + 12, 1.14e + 12$)</td>
<td>$-8.418e + 04$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$6.262e + 07$</td>
<td>($-7.054e + 11, 7.056e + 11$)</td>
<td>$-1.188e + 05$</td>
</tr>
</tbody>
</table>

### Table 17: ReZG vs. HoF.

<table>
<thead>
<tr>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 1$</td>
<td>$-4.999e + 05$</td>
<td>($-1.692e + 06, 6.922e + 05$)</td>
<td>$-5.973$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$-1.264e + 06$</td>
<td>($-4.372e + 06, 1.845e + 06$)</td>
<td>$1037$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$-7.929e + 05$</td>
<td>($-2.795e + 06, 1.209e + 06$)</td>
<td>$1486$</td>
</tr>
</tbody>
</table>
\begin{align}
\text{Entropy} (x) &= \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3}, \\
\text{Entropy} (x) &= \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},
\end{align}

where $x = R_{1/2}$ is rescaled through $\epsilon = 1117$ and $y = 945.4$.

(iv) Estimated rational polynomial of Entropy vs. $R_{1/2}$ is
\begin{align}
\text{Entropy} (x) &= \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3}, \\
\end{align}

where $x = R_{-1/2}$ is rescaled through $\epsilon = 102.3$ and $y = 81.85$.

(v) Estimated rational polynomial of Entropy vs. ABC is
\begin{align}
\text{Entropy} (x) &= \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},
\end{align}

where $x = ABC$ is rescaled through $\epsilon = 238.6$ and $y = 198.4$.

(vi) Estimated rational polynomial of Entropy vs. GA is
where $\epsilon = 365.8$ and $\gamma = 306.5$.

(vii) Estimated rational polynomial of Entropy vs. $M_1$ is

\[
\text{Entropy}(x) = \frac{p_1 x + p_2}{x^3 + q_1 x^2 + q_2 x + q_3},
\]

where $x = GA$ is rescaled through $\epsilon = 365.8$ and $\gamma = 306.5$.

(viii) Estimated rational polynomial of Entropy vs. $M_2$ is

\[
\text{Entropy}(x) = \frac{p_1 x + p_2}{x^4 + q_1 x^3 + q_2 x^2 + q_3 x + q_4},
\]

where $x = M_1$ is rescaled through $\epsilon = 2504$ and $\gamma = 2153$.
where $x = M_2$ is rescaled through $\epsilon = 4264$ and $\gamma = 3746$.

(ix) Estimated rational polynomial of Entropy vs. $\overline{M}_1$ is

\[
\text{Entropy}(x) = \frac{p_1 x + p_2}{x^3 + q_1 x^2 + q_2 x + q_3}
\]
where $x = \overline{M}_1$ is rescaled through $\varepsilon = 2.554e + 05$ and $\gamma = 3.276e + 05$.

(x) Estimated rational polynomial of Entropy vs. $\overline{M}_2$ is

$$\text{Entropy}(x) = \frac{p_1 x + p_2}{x^4 + q_1 x^3 + q_2 x^2 + q_3 x + q_4},$$

(53)
where $x = \overline{M}_2$ is rescaled through $\varepsilon = 4.283e + 05$ and $\gamma = 5.545e + 05$.

(xi) Estimated rational polynomial of Entropy vs. AZI is

$$\text{Entropy}(x) = \frac{p_1 x + p_2}{x^2 + q_1 x + q_2}. \quad (54)$$

where $x = \text{AZI}$ is rescaled through $\varepsilon = 1818$ and $\gamma = 1625$.

(xii) Estimated rational polynomial of Entropy vs. $F$ is

$$\text{Entropy}(x) = \frac{p_1 x + p_2}{x^4 + q_1 x^3 + q_2 x^2 + q_3 x + q_4}. \quad (55)$$
Figure 31: ReZG₂ vs. Entropy.

Table 20: R_i vs. Entropy.

<table>
<thead>
<tr>
<th>i</th>
<th>p_i</th>
<th>CI</th>
<th>q_i</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-2.646e+04</td>
<td>(-6.984e+04, 1.691e+04)</td>
<td>-3.384</td>
<td>(-5.642, -1.127)</td>
</tr>
<tr>
<td>2</td>
<td>-3.014e+04</td>
<td>(-7.949e+04, 1.921e+04)</td>
<td>5.483</td>
<td>(-2.395, 13.36)</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td>-473.4</td>
<td>(-1249, 302.2)</td>
</tr>
</tbody>
</table>

Figure 32: ReZG₃ vs. Entropy.

Table 21: R₁ vs. Entropy.

<table>
<thead>
<tr>
<th>i</th>
<th>p_i</th>
<th>CI</th>
<th>q_i</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-7.6e+05</td>
<td>(-4.028e+08, 4.013e+08)</td>
<td>135.2</td>
<td>(-7.287e+04, 7.314e+04)</td>
</tr>
<tr>
<td>2</td>
<td>-2.077e+06</td>
<td>(-1.1e+09, 1.096e+09)</td>
<td>-1.259e+04</td>
<td>(-6.675e+06, 6.65e+06)</td>
</tr>
<tr>
<td>3</td>
<td>-1.406e+06</td>
<td>(-7.444e+08, 7.415e+08)</td>
<td>-2.283e+04</td>
<td>(-1.208e+07, 1.204e+07)</td>
</tr>
<tr>
<td>Table 22: $R_{1/2}$ vs. Entropy.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>----------------------</td>
<td>------------------</td>
<td>------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$p_i$</td>
<td>CI</td>
<td>$q_i$</td>
<td>CI</td>
<td></td>
</tr>
<tr>
<td>$i = 1$</td>
<td>$-1.575e+06$</td>
<td>$(-1.165e+09, 1.162e+09)$</td>
<td>102.9</td>
<td>$(-7.795e+04, 7.816e+04)$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$-4.215e+06$</td>
<td>$(-3.115e+09, 3.106e+09)$</td>
<td>$-2.721e+04$</td>
<td>$(-2.013e+07, 2.008e+07)$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$-2.775e+06$</td>
<td>$(-2.049e+09, 2.044e+09)$</td>
<td>$-4.406e+04$</td>
<td>$(-3.254e+07, 3.245e+07)$</td>
</tr>
</tbody>
</table>

| Table 23: $R_{1/2}$ vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $2.454e+04$        | $(-2.946e+04, 7.854e+04)$ | $-6.267$ | $(-14.22, 1.686)$ |
| $i = 2$ | $6.443e+04$        | $(-8.139e+04, 2.102e+05)$ | 416.8 | $(-493.2, 1327)$ |
| $i = 3$ | $4.205e+04$        | $(-5.534e+04, 1.394e+05)$ | 677.3 | $(-891.1, 2246)$ |

| Table 24: ABC vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $8.579e+05$        | $(-2.287e+10, 2.287e+10)$ | 308 | $(-8.305e+06, 8.306e+06)$ |
| $i = 2$ | $2.692e+06$        | $(-7.184e+10, 7.185e+10)$ | 1.379e+04 | $(-3.674e+08, 3.675e+08)$ |
| $i = 3$ | $4.205e+04$        | $(-5.534e+04, 1.394e+05)$ | 3.185e+04 | $(-8.508e+08, 8.508e+08)$ |

| Table 25: GA vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $-5810$            | $(-1.493e+04, 3315)$ | $-3.43$ | $(-5.625, -1.235)$ |
| $i = 2$ | $-6784$            | $(-1.739e+04, 3818)$ | 5.695 | $(-2.055, 13.45)$ |
| $i = 3$ | —                  | —                  | $-108$ | $(-277.2, 61.22)$ |

| Table 26: $M_1$ vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $9765$            | $(-4.435e+04, 6.388e+04)$ | $-3.054$ | $(-8.9, 2.792)$ |
| $i = 2$ | $1.127e+04$        | $(-5.105e+04, 7.358e+04)$ | 3.672 | $(-15.14, 22.48)$ |
| $i = 3$ | —                  | —                  | $-4.83$ | $(-34.52, 24.86)$ |
| $i = 4$ | —                  | —                  | 177.9 | $(-806.6, 1162)$ |

| Table 27: $M_2$ vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $2.117e+04$        | $(421.2, 4.192e+04)$ | $-3.726$ | $(-5.577, -1.875)$ |
| $i = 2$ | $2.408e+04$        | $(522.6, 4.765e+04)$ | 378.5 | $(8.47, 748.6)$ |

| Table 28: $\bar{M}_1$ vs. Entropy. |
|----------------------|------------------|------------------|
| $p_i$    | CI                  | $q_i$ | CI                  |
| $i = 1$ | $-6.943e+06$        | $(-2.572e+11, 2.572e+11)$ | 4530 | $(-1.679e+08, 1.679e+08)$ |
| $i = 2$ | $-5.788e+06$        | $(-2.144e+11, 2.144e+11)$ | $-3.523e+04$ | $(-1.305e+09, 1.305e+09)$ |
| $i = 3$ | —                  | —                  | $-7.099e+04$ | $(-2.63e+09, 2.63e+09)$ |
where $x = F$ is rescaled through $\epsilon = 8728$ and $c = 7669$.

(xiii) Estimated rational polynomial of Entropy vs. ReZG1 is

$$\text{Entropy}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},$$

where $x = \text{ReZG}_1$ is rescaled through $\epsilon = 222$ and $c = 180.3$.

Table 29: $\mathbb{M}_2$ vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$4.171e+06$</td>
<td>$(-3.796e+11, 3.796e+11)$</td>
<td>3482</td>
<td>$(-3.171e+08, 3.171e+08)$</td>
</tr>
<tr>
<td>2</td>
<td>$3.268e+06$</td>
<td>$(-2.975e+11, 2.975e+11)$</td>
<td>$-1.149e+04$</td>
<td>$(-1.045e+09, 1.045e+09)$</td>
</tr>
<tr>
<td>3</td>
<td>$-$</td>
<td>$-$</td>
<td>$2.548e+04$</td>
<td>$(-2.319e+09, 2.319e+09)$</td>
</tr>
<tr>
<td>4</td>
<td>$-$</td>
<td>$-$</td>
<td>$4.081e+04$</td>
<td>$(-3.714e+09, 3.715e+09)$</td>
</tr>
</tbody>
</table>

Table 30: AZI vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$5.214e+06$</td>
<td>$(-1.034e+09, 1.044e+09)$</td>
<td>166.1</td>
<td>$(-3.334e+04, 3.367e+04)$</td>
</tr>
<tr>
<td>2</td>
<td>$5.886e+06$</td>
<td>$(-1.167e+09, 1.179e+09)$</td>
<td>$9.2e+04$</td>
<td>$(-1.825e+07, 1.843e+07)$</td>
</tr>
</tbody>
</table>

Table 31: $F$ vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$3.363e+04$</td>
<td>$(-1.563e+05, 2.236e+05)$</td>
<td>$-3.023$</td>
<td>$(-8.886, 2.84)$</td>
</tr>
<tr>
<td>2</td>
<td>$3.82e+04$</td>
<td>$(-1.777e+05, 2.542e+05)$</td>
<td>$3.538$</td>
<td>$(-15.1, 22.22)$</td>
</tr>
<tr>
<td>3</td>
<td>$-$</td>
<td>$-$</td>
<td>$-4.576$</td>
<td>$(-33.6, 24.45)$</td>
</tr>
<tr>
<td>4</td>
<td>$-$</td>
<td>$-$</td>
<td>$600.1$</td>
<td>$(-2788, 3988)$</td>
</tr>
</tbody>
</table>

Table 32: ReZG$_1$ vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.858e+04$</td>
<td>$(-3.576e+04, 9.292e+04)$</td>
<td>$-6.187$</td>
<td>$(-14.22, 1.843)$</td>
</tr>
<tr>
<td>2</td>
<td>$7.425e+04$</td>
<td>$(-9.781e+04, 2.463e+05)$</td>
<td>$490.1$</td>
<td>$(-606, 1586)$</td>
</tr>
<tr>
<td>3</td>
<td>$4.793e+04$</td>
<td>$(-6.582e+04, 1.617e+05)$</td>
<td>$1483$</td>
<td>$(-1054, 2590)$</td>
</tr>
</tbody>
</table>

Table 33: ReZG$_2$ vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$5.915e+04$</td>
<td>$(-7.923e+04, 1.975e+05)$</td>
<td>$-5.968$</td>
<td>$(-14.01, 2.073)$</td>
</tr>
<tr>
<td>2</td>
<td>$1.495e+05$</td>
<td>$(-2.114e+05, 5.104e+05)$</td>
<td>$1035$</td>
<td>$(-1380, 3450)$</td>
</tr>
<tr>
<td>3</td>
<td>$9.381e+04$</td>
<td>$(-1.386e+05, 3.262e+05)$</td>
<td>$1483$</td>
<td>$(-2190, 5155)$</td>
</tr>
</tbody>
</table>

Table 34: ReZG$_3$ vs. Entropy.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$p_i$</th>
<th>CI</th>
<th>$q_i$</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$8.157e+04$</td>
<td>$(3.2e+04, 1.311e+05)$</td>
<td>1448</td>
<td>$(566.3, 2329)$</td>
</tr>
<tr>
<td>2</td>
<td>$2.083e+05$</td>
<td>$(7.129e+04, 3.454e+05)$</td>
<td>2048</td>
<td>$(618.7, 3478)$</td>
</tr>
<tr>
<td>3</td>
<td>$1.311e+05$</td>
<td>$(3.961e+04, 2.227e+05)$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
</tbody>
</table>

(xiv) Estimated rational polynomial of Entropy vs. ReZG$_2$ is

$$\text{Entropy}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},$$

where $x = \text{ReZG}_2$ is rescaled through $\epsilon = 618.6$ and $c = 531.8$.

(xv) Estimated rational polynomial of Entropy vs. ReZG$_3$ is

$$\text{Entropy}(x) = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3},$$

where $x = \text{ReZG}_3$ is rescaled through $\epsilon = 222$ and $c = 180.3$. 

Complexity 23
x\_h is equally contributed by all authors. Authors' Contributions

The authors declare that they have no conflicts of interest.

ConflictsofInterest

The data used to support the findings of this study are cited at relevant places within the text as references.

DataAvailability

The authors declare that they have no conflicts of interest.

Authors’ Contributions

This work was equally contributed by all authors.

References


