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GENERALIZED ENTROPY FOR RANDOM WALKS IN REGULAR NETWORKS AND GRAPHS AS A SUPER DIFFUSION

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Abstract

In this paper, the entropy of the stochastic processes created by the movement of a walker in a graph is investigated. The Shannon-Khinchin entropy has four axioms that ignore one of them can make the generalized entropy. Here, we investigate the number of different finite paths asymptotically, for determining a generalized entropy. Then, we will study the regular infinite networks and graphs with finite nodes, with two different types of motion.

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1 Introduction

The Shannon entropy can measure the uncertainty of a random process. In probability theory, entropy is introduced by Shannon [19]. The entropy of a random variable X by distribution P taking values from a finite set E is defined by him as

$$H(X) = -E_X \log P(X) = -\sum_{i\in E} p_i \log p_i, \tag{1}$$

with the convention $0 \log 0 = 0$.

Shannon and Khinchin considered four axioms that are the main features of entropy. In the rest of this paper, we will express the generalized entropies based on these four axioms. Now, we briefly review the Shannon-Khinchin axioms.

Let Δ_W be defined by the W-dimensional simplex

$$\Delta_W = \{(p_1, ..., p_W) | p_i \geq 0, \sum_{i=1}^{W} p_i = 1\}, \tag{2}$$

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and consider $S_1(p_1, ..., p_W)$ to be the measure of uncertainty about the system.

The Shannon-Khinchin axioms [16], [20] are expressed as follows:

[SK1] Continuity: for any $W \in \mathbb{N}$, the function $S_1(p_1, ..., p_W)$ is continuous with respect to $(p_1, ..., p_W) \in \Delta_W$.

[SK2] Maximality: for a given $W \in \mathbb{N}$ and for $(p_1, ..., p_W) \in \Delta_W$, the function $S_1(p_1, ..., p_W)$ takes its largest value for $p_i = \dfrac{1}{W}$ for $i = 1, ..., W$, i.e.,

$$S_1(p_1, ..., p_W) \leq S_1(\frac{1}{W}, ..., \frac{1}{W}), \tag{3}$$

for any $(p_1, ..., p_W) \in \Delta_W$.

[SK3] Expandability:

$$S_1(p_1, ..., p_W; 0) = S_1(p_1, ..., p_W). \tag{4}$$

[SK4] Separability: If a system composed of two systems A and B that are statistically dependent, then the entropy of the composed system $S_1(AB) = S_1(A) + S_1(B|A)$ is the entropy of system A plus the entropy of system B conditional on A.

A variety of generalized entropic functionals have been introduced to phenomenologically extend statistical mechanics to specific non-ergodic or strongly interacting systems, both within and outside the realm of physics including networks [4], anomalous diffusive processes [5], time series analysis [6] and artificial neural networks [10].

The diversity of proposed entropic functionals reflects the conceptual diversity behind the assumptions all leading, in weakly correlated systems, to the same mathematical form of the Shannon entropy. In particular, arguments relying on thermodynamics, statistical mechanics, dynamical systems, information theory, and statistics all provide means to derive Shannon entropy as a useful measure, and they all provide different means to generalize it [2][12][17].

With the recent surge of interest in complex networks in various fields including statistical physics and mathematical physics, many quantities have been proposed to characterize the structural properties of graphs [8]. The study of a graph invariant in one field may also be a result of relevant importance in other areas of physics. This is because graphs are nowadays ubiquitous in many areas of physics such as in problems associated with the Ising, Potts and Hubbard models, in the solution of Feynman integrals in perturbative field theory, in quantum information theory such as quantum error correcting codes (graph states) or arrangements of interacting quantum mechanical particles (spin networks) and in many other fields [11]. Among various graph invariants, a special role has been played by the concept of entropy. Dehmer and Mowshowitz [7] have used entropy measures for graphs for a long time in different fields. Inspired by connections between quantum information and graph theory, Passerini and Severini [18] have defined the von Neumann entropy for graphs, which in general depends on the regularity, the number of connected components, the shortest-path distance and nontrivial symmetries in the graph.

Here, we define graph entropies based on walks in a graph. Walks in graphs play a fundamental role in the analysis of the structure and dynamical processes in networks [9]. The walk entropies thereby characterize the spread of a walk among the vertices or edges of the graph.

Before proceeding, we summarize a few definitions which are necessary to make this paper self-contained. Let us consider here simple graphs $G = (V, E)$ with $|V| = n$ nodes and $|E| = m$ edges. A walk of length k is a sequence of (not necessarily distinct) nodes $v_0, v_1, ..., v_k$ such that for each $i = 1, 2, ..., k$ there is a link from v_{i-1} to v_i. The number of walks of length N from node p to node q is given by $[\mathbf{A}^N]_{pq}$ (the element of row p and column q of matrix $\mathbf{A}^N$), where $\mathbf{A}$ is the adjacency matrix of the graph G. The degree of the node p , denoted by p_k , is the number of edges incident to it.

In order to define graph entropies based on the walks, we consider a random walker which walks from one node to another by using the edges of the graph.

This paper is organized as follows: Section 2 discusses extensive or generalized entropies that one can see more details in [14]. In this section, the four axioms of Khinchin, whose unique result is Shannon's entropy, are outlined. By ignoring the fourth axiom, one can obtain the general form of extensive entropies that depend on two parameters (c, d). Section 3 contains four examples. In this section, we examine two different types of motion in $\mathbb{Z}^D$ and graphs. In the first case, at each step there is a choice of a new direction for the walker, while in the second case, after selecting a direction for walking , the change of direction is not possible for a finite number of next steps.

2 Review of generalized entropies

Shannon and Khinchin showed that, assuming four information theoretic axioms, the entropy must be of the Boltzmann-Gibbs type, $S = -\sum_i p_i \log p_i$, in the following uniqueness theorem.

Theorem 1. *: Let $S_1(p_1, ..., p_W)$ be a function defined for any integer $W \in \mathbb{N}$ and for any $(p_1, ..., p_W) \in \Delta_W$. If for any $W \in \mathbb{N}$ this function satisfies the properties [SK1]-[SK4], then*

$$S_1(p_1, ..., p_W) = -k \sum_{i=1}^{W} p_i \log p_i, \tag{5}$$

where k is a positive constant.

Proof. The proof of this uniqueness theorem is given in [16]. □

There are entropies that do not necessarily satisfy all Shannon and Khinchin axioms. These results were previously proven in [1]. These entropic forms are called generalized entropies and usually assume trace form, e.g. in [21]

$$S_g(p) = \sum_{i}^{W} g(p_i) \tag{6}$$

where W is the number of states. For example the Tsallis entropy with the following formula is one of the generalized entropies[21].

$$S_q(p) = \frac{1 - \sum_i p_i^q}{1 - q}, \tag{7}$$

where, we can assume that $g(p_i) = \dfrac{p_i - p_i^q}{1 - q}$.

Obviously not all generalized entropic forms are of this type. Renyi entropy is of the form, $G(\sum_i^W g(p_i))$, with G a monotonic function. We use trace forms Equation (6) for simplicity. Renyi forms can be studied in exactly the same way, as will be shown, however, at more technical cost.

As mentioned, if all of Shannon and Khinchin axioms hold, the only possible entropy is the Boltzmann-Gibbs-Shannon (BGS) entropy. The generalized entropy for (large) admissible statistical systems (all of Shannon and Khinchin axioms except separability axiom hold) is derived from two hitherto unexplored fundamental scaling laws of extensive entropies [12]. Both scaling laws are characterized by exponents c and d, respectively, which allow one to uniquely define equivalence classes of entropies, meaning that two entropies are equivalent in the thermodynamic limit if their exponents (c, d) coincide. Each admissible system belongs to one of these equivalence classes (c, d), [12]. In terms of exponents (c, d), Hanel and Thurner [12] showed that all generalized entropies have the form

$$S_{(c,d)} \propto \sum_{i=1}^{W} \Gamma(d + 1, 1 - c \log p_i) \tag{8}$$

with

$$\Gamma(\mu, t) = \int_t^\infty y^{\mu-1} e^{-y} dy = \int_0^{e^{-t}} (-\ln x)^{\mu-1} dx. \tag{9}$$

Also, $\Gamma(\mu, t)$ named the incomplete Gamma-function and μ is a complex parameter, such that the real part of μ is positive.

2.1 Determining the exponents, c and d

Consider a system with N elements. The number of system configurations (microstates) as a function of N is denoted by $W(N)$. In [13], Hanel and Thurner proved that:

$$\frac{1}{1 - c} = \lim_{N \to \infty} N \frac{W'(N)}{W(N)} \tag{10}$$

and

$$d = \lim_{N \to \infty} \left[\frac{W(N)}{NW'(N)} + c - 1 \right] \log W(N) \tag{11}$$

Here, W' means the derivative with respect to N.

3 Some different random walks in graphs

A lattice path L in $\mathbb{Z}^D$ of length k with steps in S is a sequence $v_0, v_1, ..., v_k \in \mathbb{Z}^D$ such that each consecutive difference $v_i - v_{i-1}$ lies in S. Now we consider S as a set of $(x_1, x_2, ..., x_D) \in \mathbb{Z}^D$ such that exactly one of x_is is 1 or -1 and others are 0, i.e.

$$S = \{(1,0,...,0), (-1,0,...,0), (0,1,...,0), ..., (0,0,...,0,-1)\}. \tag{12}$$

3.1 Random walks in $\mathbb{Z}^D$ uniformly

Suppose that a walker can choose one member of S as a direction for walk in each step. If the transition probability of this process is

$$Pr(v_i = k|v_{i-1} = j) = \begin{cases} \frac{1}{2D} & k - j \in S \\ 0 & k - j \notin S, \end{cases} \tag{13}$$

then, there are $W(N) \sim (2D)^N$ difference paths with length N.

Proposition 1. *For random walk on* $\mathbb{Z}^D$*, with transition probability uniformly* (13)*, the parameters* $(c, d) = (1, 1)$*.*

Proof. In this case using (10) and (11), we can obtain

$$\begin{aligned} \frac{1}{1-c} &= \lim_{N\to\infty} N \log(2D) = \infty \Rightarrow c = 1, \\ d &= \lim_{N\to\infty} N \log(2D)\left(\frac{1}{N\log(2D)} + c - 1\right) = 1. \end{aligned} \tag{14}$$

□

So, this random walk has Shannon entropy. Note that this process is a Markovian process. Interestingly the continuum limit of such processes is well defined.

3.2 Random walks in $\mathbb{Z}^D$ as a super diffusion

Now we study super diffusion in $\mathbb{Z}^D$ as a non Markovian process. The particular case of $D = 1$ is discussed in [13]. Consider a walker choose a member of S as a direction for moving in step N(N being the total number of steps the walker has taken so far). He has to follow this direction by $\lceil N^\beta \rceil$ consecutive steps, where $\lceil\rceil$ means rounded to the next higher integer (the ceil operator) and $0 \leq \beta < 1$. In other words, if after N timesteps, a walker choses a node from S, this selection will be kept for the next $\lceil N^\beta \rceil - 1$ steps. At timestep $N + \lceil N^\beta \rceil$ the next free decision is possible. For example, consider $\beta = 0.5$. At step $N = 1$ the random walker decides to go one of $2D$ possible directions, e.g. $w(1) = (1, 0, ..., 0) \in S$. He has to continue to go in this direction for $\lceil 1^{0.5} \rceil = 1$ steps. At $N = 2$ he freely decides to go in another direction, e.g. $w(2) = (0, 1, ..., 0) \in S$. He now has to continue to go in this direction for $\lceil 2^{0.5} \rceil = 2$ steps, i.e. $w(3) = w(2) = (0, 1, ..., 0)$.

At $N = 4$ he can decide again, and so on. After N steps the walker is at position $x_\beta(N) = \sum_{n=1}^{N} w(n)$. Clearly, the number of decision grows like $N^{1-\beta}$, and the number of possible sequences $W(N) \sim (2D)^{N^{1-\beta}}$. Consequently the associated extensive entropy is of class $(c,d) = (1, \frac{1}{1-\beta})$ because,

Proposition 2. *For super diffusion in $\mathbb{Z}^D$, as described above, the parameters $(c,d) = (1, \frac{1}{1-\beta})$.*

Proof. Proof of this proposition is possible with relations (10) and (11). we have

$$\begin{aligned}
\frac{1}{1-c} &= \lim_{N\to\infty}(1-\beta)N^{1-\beta}\log(2D) = \infty \Rightarrow c = 1, \\
d &= \lim_{N\to\infty} N^{1-\beta}\log(2D)\left(\frac{1}{(1-\beta)N^{1-\beta}\log(2D)} + c - 1\right) = \frac{1}{1-\beta}.
\end{aligned} \tag{15}$$

□

3.3 Random walk in Graph $G(V,E)$

We now focus our discussion on random walks in undirected graphs with uniform edge weights, with no multiedges or self loops. At each node, the random walk is equally likely to take any connected edges. Assume the graph $G = (V,E)$ with $|V| = n$ nodes and $|E| = m$ edges, is connected. On the other hand, since the graph G is connected, one can find an integer k such that all of entries $\mathbf{A}^k$ are positive, where $\mathbf{A}$ is the adjacency matrix of the graph. We know the number of walks of length N i.e. $W(N)$ from node p to node q is given by $[\mathbf{A}^N]_{pq}$.

Proposition 3. *For random walks in undirected graphs, as described above, , the parameters $(c,d) = (1,1)$.*

Proof. It is necessary to express spectral representation of matrices and Perron-Frobenius theorem. We use the spectral representation [15] of the matrix $\mathbf{A}$. Since $a_{ij} \geq 0$, and there is an integer k such that $[\mathbf{A}^k]_{ij} > 0$, the Perron-Frobenius theorem [3] applies. So there exists a real eigenvalue λ_1 with algebraic geometric multiplicity one such that $\lambda_1 > 0$, and $\lambda_1 > |\lambda_j|$ for any other eigenvalue λ_j. Moreover the left eigenvector l_1 and the right eigenvector r_1 associated with λ_1 can be chosen positive and such that $l_1 r_1^t = 1$.

Let $\lambda_2, \lambda_3, ..., \lambda_m$ be the eigenvalues of the $\mathbf{A}$ other than λ_1 ordered in such a way that $\lambda_1 > |\lambda_2| \geq |\lambda_3| \geq ... \geq |\lambda_m|$ and we know that the vectors r_1 and l_1 are real-valued with nonnegative components. The matrix spectral representation yields

$$\mathbf{A}^N = \lambda_1^N(r_1^t l_1) + |\lambda_2|^N(r_2^t l_2) \Rightarrow \mathbf{A}^N = \lambda_1^N(r_1^t l_1) + o(|\lambda_2|^N). \tag{16}$$

We can consider

$$|\lambda_2|^N(r_2^t l_2) = o(|\lambda_2|^N), \qquad \lambda_1^N(r_1^t l_1) = o(\lambda_1^N), \tag{17}$$

so

$$\mathbf{A}^N = \lambda_1^N (r_1^t l_1) \left(1 + o\left(\frac{|\lambda_2|^N}{\lambda_1^N}\right)\right). \tag{18}$$

Now we know the number of walks of length N from node p to node q is given by $[\mathbf{A}^N]_{pq}$, so $W(N) \sim \lambda_1^N (r_1^t l_1)_{pq}(1 + o(\rho))$ where $\rho = (\frac{|\lambda_2|^N}{\lambda_1^N}) < 1$. One can obtain

$$\begin{aligned}
\frac{1}{1-c} &= \lim_{N\to\infty} N \log \lambda_1 = \infty \Rightarrow c = 1, \\
d &= \lim_{N\to\infty} [N \log \lambda_1 + \log(r_1^t l_1)_{pq}(1 + o(\rho))](\frac{1}{N \log \lambda_1} + c - 1) = 1.
\end{aligned} \tag{19}$$

□

So $(c, d) = (1, 1)$ and this random walk in graphs has Shannon entropy.

3.4 Random walk in Graph $G(V, E)$ with self loop

We now focus our discussion on random walks in undirected graphs with uniform edge weights. At each node, the random walk is equally likely to take any edge. Now suppose the graph has self loop with probability weight zero. A super diffusion walk in this graph is described as remaining in the same node for $\lceil N^\beta \rceil$ timesteps after selecting an edge in step N. In other words, the walker moves on self loop without making any new decisions and the next free decision is possible at timestep $N + \lceil N^\beta \rceil$. Clearly, the number of decision grows like $N^{1-\beta}$, and the number of possible sequences without considering self loops, is related to $\mathbf{A}^{N^{1-\beta}}$, therefore

$$W(N) \sim \lambda_1^{N^{1-\beta}} (r_1^t l_1)_{pq}(1 + o(\rho)), \tag{20}$$

where here $\rho = (\frac{|\lambda_2|^{N^{1-\beta}}}{\lambda_1^{N^{1-\beta}}}) < 1$.

Proposition 4. *The associated extensive entropy, as described in this subsection, is of class* $(c, d) = (1, \frac{1}{1-\beta})$*, because*

Proof. using (10), (11) and (20), we can obtain

$$\begin{aligned}
\frac{1}{1-c} &= \lim_{N\to\infty} (1-\beta) N^{1-\beta} \log \lambda_1 = \infty \Rightarrow c = 1, \\
d &= \lim_{N\to\infty} [N^{1-\beta} \log \lambda_1 + (1-\beta) \log(r_1^t l_1)_{pq}(1 + o(\rho))] \\
&\quad \times (\tfrac{1}{(1-\beta) N^{1-\beta} \log \lambda_1} + c - 1) = \tfrac{1}{(1-\beta)}.
\end{aligned} \tag{21}$$

□

4 Numerical example

Now, for the two graphs **A** and **B** shown in Figure 1, the walker movement diagram on Graph **A**, with 100 and 10,000 time-steps, is shown in Figures 2 and 3, respectively. Similarly, Figures 4 and 5 correspond to Graph **B**.

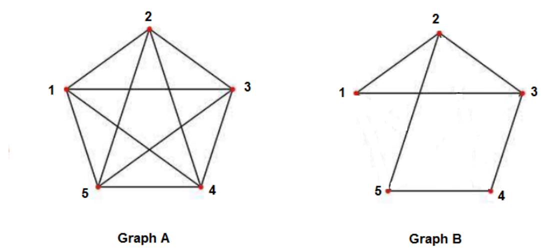

Figure 1: Two graphs **A** and **B**

In each figure, the upper diagram is related to the simple walk, and the lower diagram is related to the super diffusion walk.

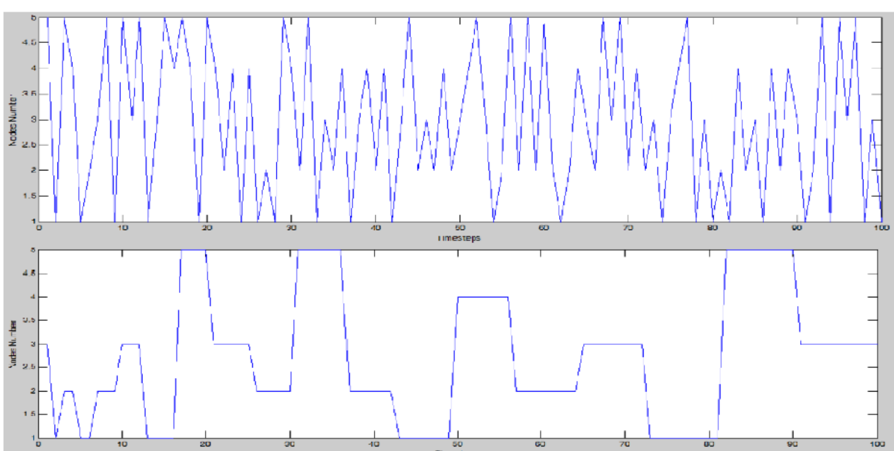

Figure 2: The upper diagram is related to the simple walk, and the lower one is related to the super diffusion walk for 100 time-steps on Graph **A**

It can be seen that these two types of movements are completely different. As expected, we showed that their entropies are also different.

Conclusion

We studied the relationship between the volume of state space of a stochastic process and its extensive (generalized) entropy. If the volume of state space Ω is given as a function of system size, we are know how to determine the associated generalized entropy by computing the parameters (c, d). We demonstrated in four

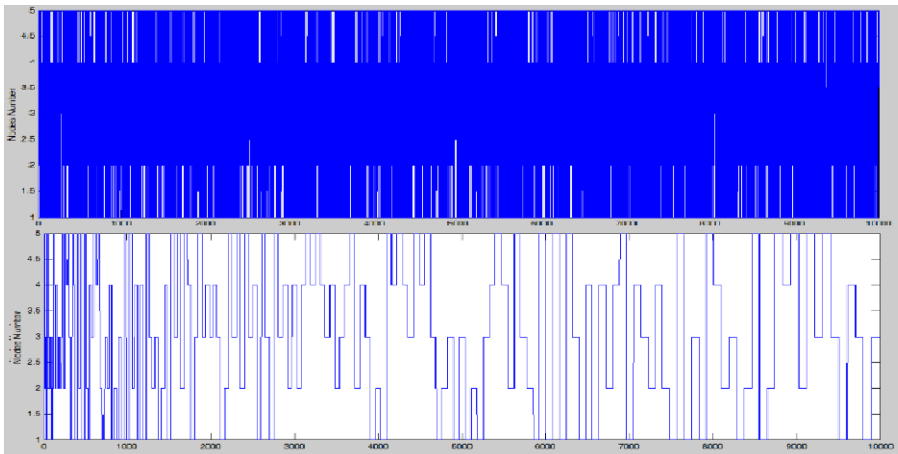

Figure 3: The upper diagram is related to the simple walk, and the lower one is related to the super diffusion walk for 10000 time-steps on Graph **A**

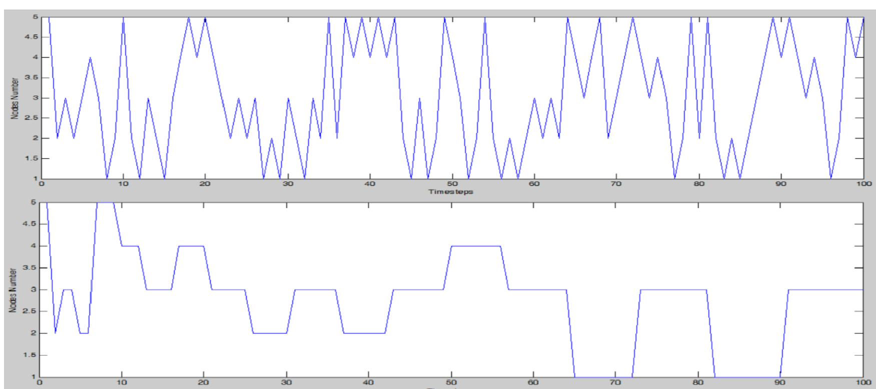

Figure 4: The upper diagram is related to the simple walk, and the lower one is related to the super diffusion walk for 100 time-steps on Graph **B**

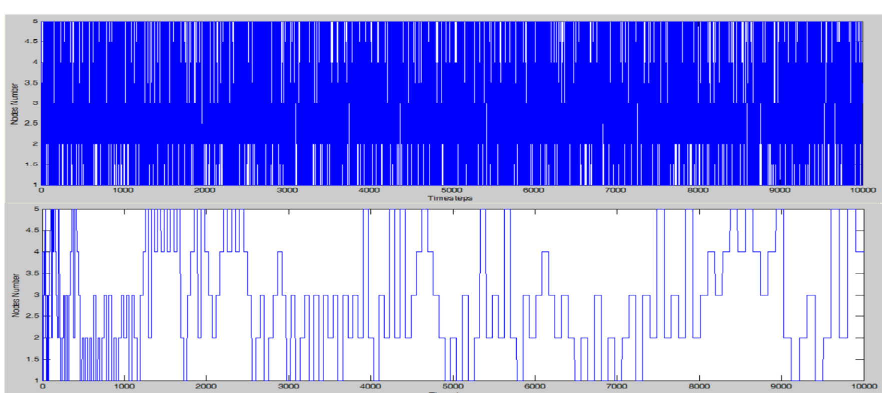

Figure 5: The upper diagram is related to the simple walk, and the lower one is related to the super diffusion walk for 10000 time-steps on Graph **B**

concrete examples how statistical systems determine their own extensive entropies. All four examples are simplifications of more general real-world situations. In the first example, a walker moves in a D-dimensional network, where he can select one of the nodes around himself in each step to move, uniformly. Sometimes, conditions in a statistical system can limit mobility in Euclidean space. The second example proposed a particular type of these conditions and calculated the parameters (c, d) for associated generalized entropy. This kind of random motion in Euclidean space does not fall into the category of Markovian processes. The third and fourth examples examine the motion of a walker in undirected and connected graphs. In the third example, as in the first example, the walker selects the next node for displacement, from set of the possible nodes, at any time-step uniformly. In the fourth example, the walker selects a new node for movement and stays on his new place for a certain number of time-steps moving on its self loop, meaning that after several time-steps, the walker goes to another node. In the first and third examples that the certain kind of the Markov chains were shown, we obtained their generalized entropies as the same as the Shannon entropy. Whereas in the second and fourth examples where non-Markovian processes were investigated, their generalized entropies were not the Shannon entropy.

Many issues remain to be investigated. One interesting extension is the mutual information for generalized entropies and another is the generalized entropy rate of stochastic processes.

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