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Entropy in Dynamical Networks

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Abstract

This thesis presents a new type of dynamical entropy, defined by the movement of particles beetween the nodes in a network. The entropy is intended to have similar properties as the well-known thermodynamic entropy. Simulations are run on different versions of known networks, and exhibits expected behaviour. A few applications of the variable have also been suggested, in which topographical properties, centrality and node distance is decided in relative terms for spesific networks. In addition, a historical recap is the science of thermodynamics and networks is given, and also an explanation to how these fields have come together over the recent years, culminating in this effort to further connect them.

Sammendrag

Denne masteroppgaven presenterer en ny type dynamisk entropi, definert for bevegelse av partikler mellom nodene i et nettverk. Entropien er tiltenkt å ha lignende egenskaper som den velkjente termodynamiske entropien. Det er kjørt simuleringer på forskjellige versjoner av kjente nettverk, og entropien oppfører seg slik som ventet. Noen applikasjoner av variabelen har også blitt foreslått, der de topografiske egenskapene sentralitet og nodeavstand har blitt bestemt relativt for spesifikke nettverk. I tillegg til dette er det gitt en historisk oppsummering av feltene termodynamikk og nettverksvitenskap, en forklaring på hvordan disse feltene har sammenfalt i de senere år, og tilslutt hvordan dette har kulminert i dette forsøket på å forene de ytterligere.

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Preface

This document is my thesis for the Masters degree program Technical Physics at the Norwegian University of Science and Technology (NTNU), carried out in the period October 2012 - March 2013.

I would like to extend my deepest gratitude to my supervisor Professor Ingve Simonsen, and to Associate Professor Peter Berg. Both have shown a great interest in my work, and have provided extensive amounts of time for hours long, interesting and fruitful discussions every time I had a question. Their dedication and love for the sciences have truly been inspiring, and have played a big role in motivating me.

I would also like to thank my fellow students during my studies, which many of them have become some of my closest friends and confidants over the last years. The effort of a 5 year study has been made easy by the constant activity surrounding us, from playing games, excersising, cooking, partying, discussing, vacationing and cohabitational activities. In the fear of forgetting someone, I won't mention anyone by name, but I thank you all from the bottom of my heart. You know who you are.

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Contents

List of Figures

Chapter 1

Introduction

In an increasingly complex, digitalized and interconnected world, the studies of network have become more and more interesting. Whether they are used to directly represent your friendsships on a social network site, or used more abstract to model intercity aviation traffic, networks can be very helpful to visualize and concretizise abstract entities. The advent of the computer allows us to explore problems with a complexity hereto unaccessible, allowing for modelling and simulations of increasingly complex networks. These networks have the interesting feature that any behaviour modeled on them will be affected by many different features of the network, both by the restrictions in the network and the way the network is connected. One could consider the internet, which is in many ways the network that is most obvious to us in our daily life. The way in which information spreads here, is not given in itself by the computational power of each individual computers, but rather by the choises of the people using the computers and how the computers are interconnected in a network. In the neural networks of our brain, it is possible to understand the function of each neuron by itself, and we know a lot about how each of them stores and emits information. It is yet, however a mystery how the connections of a large number of these can give rise to the complexity that is our mind and the thought processes. Indeed, Aristoles famous notion that "The whole is greater than the sum of its parts" is repeatedly proving to be an inherent rule of the natural systems.

With the increasing complexity, the idea of how one works with these models has changed, as one no longer necessarily can assess all information by merely eyeballing networks, but rather must construct tools to analytically treat them. The same concept has earlier been applied to a lot of real world problems, and one of the most successful fields has been the science of thermodynamics. Here, huge models of directly uncomputable size has been simplified by considering the statistical properties of the constituents as an ensemble, instead of doing direct computations on one and one particle. In this thesis, we will attempt to take one of the most important in the science of thermodynamics, namely entropy, and introduce into the science of networks. Doing this, we hope to transfer some of the work that has already been done and applying it to a new field.

Chapter 2

Theory

2.1 Entropy

Two of the most fundamental principles in physics is stated in the first and second law of thermodynamics. Both of them have been expressed by several sources and in several ways, but the essence of them is as follows; The first law states the principle of energy conservation in a process. It says that in a thermal process, all internal energy exchange from a system to it's environment must result in a corresponding amount of work or heat exchange. The second law makes a statement about the preferred direction of processes, namely that heat will always move from a warm object towards a colder, thereby seeking an equilibrium. This is opposed to the impossible scenario where the cold object would become even colder to further enhance the temperature of the warmer[1].

2.1.1 Macroscopical Entropy

In the middle of the 19th century, after the industrial revolution had made its everlasting impact on the western world, steam engines were to be found in every modern industry. As more and more steam engines came into use,

the coal used as fuel became a commodity, and the prices rose. It was in these times the german physicist Rudolf Clausius discovered the principles of entropy while he was working on determining the maximal efficiency of steam engines, expanding on the earlier work of Carnot. Clausius' work was based on the derivations of how the macroscopic quantities temperature, work and heat of systems behaved when undergoing idealized Carnot cycles, These derivations combined with the axiom that "Heat cannot pass by itself from a cold to a hot body" [2] led to the definition of the state-function, S, called *Entropy*. Clausius' definition of entropy was closely connected to thermal systems undergoing theoretical circuit processes. It was also only defined for the relative difference in entropy of a system in two different states. Clausius' macroscopically founded definition of the difference in entropy between two states A and B, is given as

$$S_B - S_A = \int_A^B \frac{dQ_{\text{rev}}}{T},$$

or in the differential form,

$$dS = \frac{dQ_{\text{rev}}}{T}. \tag{2.1}$$

In both cases, Q_{rev} is the heat exchanged between the system and its environment through a reversible circuit process, whereas T is the temperature of the reservoir where the system deposits or withdraws heat. The unit for entropy is [J/K].

Further exploration on this new concept of entropy led to a reformulation of the laws of thermodynamics. The reformulated laws stated by Clausius was "The energy of the world is constant, and its entropy strives towards a maximum. [1]" Another more precise formulation of the last part is that "the entropy of an isolated system never decreases, because isolated systems spontaneously evolve towards thermodynamic equilibrium". In mathematical terms this is expressed as

$$\frac{dS}{dt} \geq 0, \tag{2.2}$$

where S is the entropy of the system.

From pure macroscopic phenomena, Clausius was able to discover entropy as the driving force of thermal processes. In order to get a deeper and more fundamental understanding of the phenomenon, an understanding of the microscopic mechanics involved was needed.

2.1.2 Microscopical Entropy

In the middle of the 19th century, the scientific community considered the macroscopic variables such as temperature and pressure to be the results microscopic phenomena. This idea was first postulated by Bernoulli in his work *Hydrodynamica*, which he published in 1738. In the book, he attributed heat and pressure of gases to the movement of great numbers of molecules. Heat was simply the accumilated effect of these molecules' kinetic energy, and pressure was the collective impact of the molecules on a surface. This idea had been further explored by the already mentioned Clausius, whose work on diffusion led Maxwell to discover the famous Maxwell distribution of molecular velocities. This was the first statistical law in physics and laid the way open for a whole new branch of physics. It was the starting point for both statistical mechanics and the career of the young austrian Ludwig Boltzmann. He went on to spend the greater part of his career laying the groundwork for the dicipline of statistical mechanics, and his greatest contribution in that respect is considered by many to be the microscopic definition of entropy. He considered a given system to simultaneously be in both a macrostate and a microstate. The macrostate was the traditional view of macroscopical variables, with a given pressure, temperature and volume. The microstate was the more accurate description of the single particles, including position and velocity for each and every one of them. For each macrostate, there could be a huge amount of corresponding microstates which would give the same macroscopical variables. The number of corresponding microstates to a given macrostate, Ω, is together with k_B, the Boltzmann constant, the key part of the Boltzmann entropy[1],

$$S = k_B \ln \Omega. \tag{2.3}$$

The claim that this was the most important piece of work Boltzmann did, is supported by the fact that this is what is engraved on his gravestone in Vienna. This Boltzmann entropy asserted the fact that the entropy had a logarithmic relation to some probability of the occurance of the state. The number Ω is directly proportional to the probability of a macrostate, as the number of microstates is higher for macrostates with a higher probability. The Boltzmann entropy requires, however, an important assumption that prohibits universal validitiy; that all microstates were equally probable, which only holds true for ideal gases.

An important property of entropy worth mentioning at this point is what happens with the entropy when two ideal, non-reactive gases are mixed. Imagine a setupone initially has two gases in a container, each with its own entropy, and separated by a barrier. When the barrier is removed, the entropy of the whole system will be larger than for the sum of the two gases initially, due to a larger uncertainty of position[1]. This important attribute of entropy will be further studied later in this thesis.

2.1.3 Probabilistic Entropy

In order to generalize Boltzmann's entropy, the assumption of equal probability for all microstates had to be removed. This was done by simply weighing each of the microstates with a probability, and then summing over all the states. This was done by Josiah Willard Gibbs, and it bears the name Gibbs entropy. The new extended formula for entropy was [3]

$$S = -k_B \sum_i p_i \ln p_i,$$

where p_i is the probability for microstate i to occur. The negative presign is to ensure a positive entropy when the log of a probabillity, $p \leq 1$ produces a negative sign. For ideal gases, where all probabilities are equal, the formula reduces to Boltzmanns entropy (2.3). The formula has been proven to yield numerical results equal to Clausius' experimental entropy

(2.1) [4], thereby successfully combining the microscopical and macroscopical both quantitatively and qualitatively.

Through these equations, the understanding of the nature of the entropy developed. From an initial constructed variable with no deeper explanation beyond the works of a steam-engine, a profound understanding about the ways of nature was derived. The most important aspect in most eyes was the way in which entropy made it possible to observe and measure the second law of thermodynamics directly, giving all physical reactions a "purpose" and directions. This was widely discussed, not only in physics, but also in other areas such as philosophy and religion, where it was a strong point for the determinists who believed the whole story of the universe was set and just performing according to preset rules before our eyes. The champions of these views did indeed have a very strong argument, at least until the peculiarities of quantum physics was discovered. (Indeed, as von Neumann later would discover, the entropy is well defined also for quantum systems)

In later years, entropy has been further generalized by the Brazilian physicist Constantino Tsallis. In the same manner that newtonian mechanics are not valid for velocities near the speed of light, the Boltzmann-Gibbs entropy has been found to not hold for nonextensive systems, i.e complex systems where the components has a high degree of correlation between them. The new generalized formula is [3]

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

where q is a real parameter called entropic-index, and $\{p_i\}$ is a discrete set of probabilities. in the limit $q \to 1$, we get the Boltzmann-Gibbs entropy.

2.1.4 Entropy Outside of Physics

Among those lesser inclined to ponder on the big questions in life, there was also a grand interest for the concept of entropy and the uses of it in

other branches of science apart from thermodynamics. One of them was the brilliant young engineer Claude E. Shannon. He had written a brilliant master thesis on boolean logicals, and after working with cryptography at the Bell laboratories during World War II, he was ready to start the new branch the science called information theory.

Shannon started looking at the "bit", the information carrier in a digital computational system. He set out to find a way do encode information in the most efficient way thorugh "bits", and did so by introducing a set of new concepts. One of these was the notion of uncertainty of information. He argued that for a set of outcomes where the probabilities were not equal, the uncertainty was lower that for a set where every outcome was just as likely. This uncertainty was quantified through the formula[5]

$$H(X) = P(x_i) \log_b(P(x_i), \tag{2.4}$$

where H is the uncertainty, $X = x_1, x_2....x_n$ is the set of outcomes, and $P(x_i)$ is the probability for outcome x_i. The base of the logarithm is set by the information carrier size. If it is a bit, $b = 2$. By comparing his uncertainty idea with Boltzmanns entropy, it was evident that there was an analougue between the two notions. In the statistical mechanical entropy, the notion of uncertainty is represented in the value Ω, where a higher value would mean a higher number of microstates for the given macrostate, i.e a higher uncertainty about which microstate it actually was. As the concepts and the equations, (2.3) and (2.4), were similar, Shannon decided to call this uncertainty entropy.

Shannon was not the only one who made use of the concept of entropy in branches seemingly unrelated to physics. After the initial coining of the term, it has been put to use in a wide range of fields including, but not limited to, economics [6], sociology [7], medicine [8] and ecology [9].

2.2 Networks

2.2.1 The Seven Bridges of Königsberg

The science of networks, in mathemathical terms referred to as Graph theory, was initiated by the publication of mathemathician Leonard Euler's 1736 paper "The Seven Bridges of Königsberg". The problem he treated was whether it was possible to cross all seven bridges in the Prussian city Königsberg without crossing each bridge more than once. He concidered the problem, and realized it would be a lot easier to work on the problem if he removed all the unimportant information of the problem, so he simplified the islands and land sides into dots and the bridges into lines. What he had constructed is what i mathematical terms is called a *graph*. By just considering the simple graph he had made, he drew the conclusion that the feat had to be deemed impossible, as there were more than two nodes with an odd number of links connected to it. The idea is that the start- and end-nodes could have odd numbers, but an odd number on any of the other nodes, would lead to a stop, as there are more ways in than out. The remarkable aspect of his solution was the way he simplified the problem from the real world into a mathemathical construct called a graph, allowing for analytical and logical treatment.

Figure 2.1: Eulers simplification of the problem of the bridges of Königsberg. On the left is an illustration of the actual city layout, in the center a more simplified version, and on the right the problem is described through a graph. Figure taken from [10]

2.2.2 Networks in Social Studies

After the initial work by Euler, it took quite some time before mathematicians further developed a science around networks. Networks were instead much more in use to represent connections in social sciences, biology, and other sciences where the network is given inherently by the studied structures. The size of the networks were often so small that constructing them visually and get information just by using eyesight was possible. The Karate network studied by Zachary is a good example of the types of networks studied in the middle of the 20th century, where social groups were mapped through censuses and observations of structure were made from the visualization. This network will be presented in further detail, and studied later in this thesis.

A famous social study network was performed by Stanley Milgram in 1967. It was believed at the time that all people in the world was connected to each other in a closely connected network. From general assumptions about how many friends each individual has in average, it had been calculated that six steps of separation would be sufficient to link any individual on the earth to any other. The huge network this theory regarded, with approximately 3.5 billion nodes, and a much higher number of links, was at this point, and still, impossible to construct, and study accurately. Even at this point in time, where social networks are automatically digitalized on portals such as Facebook, and our computational abilites have sky-rocketed, it is not yet possible to confirm or reject this hypothesis definetly. Milgram was well aware of the impossibility, but still designed an experiment to give an indication as to whether the theory was correct. He chose a number of individuals in the United States at random and sent them a package with instructions. The goal was that they should send a package to a named person in as few steps as possible. They were given some information about the target, and the rule that they were only allowed to send the package to people they knew. If they did not know the target, they were to try to guess which of their friends had the closest relation to the target, and to send them the same instructions. A lot of packages never reached the target, but a sufficient amount did, and the results indicated that indeed, the idea of a six step separation was deemed

reasonable. This experiment was ground-breaking in that it could say something about the network as a whole without having to have complete information about the network. This treat of networks where the number of nodes vastly outnumber the average degree distribution is in general called *the small world phenomenon.*

2.2.3 Networks in Mathematics

Intrigued by the information gained from such experiments as Milgrams, and the possibility of expanding the knowledge into the natural sciences, the interest of networks grew tremendously among mathematicians. In 1959, the two hungarians Paul Erdős and Albért Rényi constructed an algorithm to construct random networks, and continued to explore general properties to classify networks[11][12]. They defined properties like degree-distribution and fractioning for any network. The degree of a node is given by the amount of links it has to other nodes. A degree distribution analyses the whole network and gives the relative occurence for each degree. Fractioning is a property that represents to which degree the whole network is connected or, i.e. any given node is connected to all the others through links. Related is also the geodesic distance between two nodes, which is the shortest amount of links one has to traverse in order to get from one node to another by traversing through the network.

Comparing the work done by the Erdős and Rényi to the growing number of real-world networks studied, gave rise to some problems. Their completely random network construction did in fact not seem to give the kinds of networks that was generally found when real-world networks was studied. For instance, the Erdős-Rényi networks had a Poisson-distribution of the degrees, whereas networks in the real world tends to have a power-law distribution. The occurence of a topgraphical property called clustering was also observed everywhere in the real world, but not in Erdős-Rényi networks. Clustering is the phenomena that a group of nodes are tightly bound with each other, but only connected at a few points to the rest of the network. A real-world example could be a city with several schools,

where the students in general have most of their friends at their school, thereby making a cluster in the social network. The small world phenomenon was also generally not present. The mismatch between what was observed and complete randomness indicated that there were some rules as to how networks grew.

Two pairs of mathematicians came up with different solutions to the mismatch in a short time span. in 1998, Duncan J. Watts and Steven Strogatz made an algorithm that took a random network and changes connections to make clusters[13]. This expansion on Erdős-Rényi networks made networks more similar to what was found in the real world, including both clusters and small world phenomena. Still, the degree distribution is not changed, and the incompability is still present. Another problem with this model is that it does not account for growing networks, i.e. networks where the number of nodes grow, which is the case for countless networks in the real-world. Albert László Barabási and Réka Albert came out with a different approach in 1999[14]. Starting with a small network, new nodes are added and connected in a manner called preferential attachment. The idea is that any new node that is connected to the network has a higher probability of connecting to nodes that already have a high degree. This is thought to be anologous to the process in which real social networks grow, where it is generally easier to get to know people that already have a lot of contacts, as they tend to be more social, and also because the chance of being introduced to them by a third party is higher than to someone that has fewer connections. These networks give rise to power law distribution of degrees, but has shortcomings when it comes to producing a high level of clustering. This is due to the fact that the connections are chosen indiscriminately of group belongings, and therefore, if there at some point happens to be clusters, the chances of connecting said clusters to each other are high, which will in turn remove them.

2.2.4 Networks in Physics

A network is in this thesis defined as a number of objects connected to each other in a specific manner. The objects are defined as nodes, and the connections as links. The networks can be interconnected in several different ways, which in turn leads to very different network behaviour. For instance can the connections be directed or undirected. In the undirected network, the connection between two nodes is completely symmetrical and equal for both nodes. For a real world example, one can consider the friend network on social network sites like Facebook. If a person A is in the friend list of a person B, then by the construct of the site, person B will have to also be in person A's friend list. In an undirected network, the connection from A to B does not necessarily imply the connection from B to A. An example of this can be a someones phone book or contact list. Even though most of the numbers would have come into the phone book after some mutual exchange, it can also be the case that the number has been given by a third party or found online. For another examples from the area of social networks, one can look at "Twitter". Here, the relationship between two parties are directional, and separeted with the notion of either "following" someone, or "being followed". In this thesis, the more general notion of directed networks will be used even though the results presented mostly concerns undirected.

Networks can also be divided by the notions *weighted* and *unweighted*. These terms allows for distinguishing between strong and weak connections between nodes, for instance in a computer network, where the traffic between two computers connected on a Local Area Network, can be much larger then two computers connected through the internet. Another example is to simulate a transport network, where nodes are intersections and links are roads. The weight of the link can represent a highway, the weight being proportional to the number of files on the road, and/or the length of a road, the weight being inverse proportional to the length and/or the speed limit of the road.

In order to represent a network, it is common to use and Adjecency matrix, A. This is a $n \times n$ matrix where the term A_{ij} represents the directed connection from $j \to i$. The indices represents the n nodes, so that $i, j \in \{1, 2, ..., n\}$. The Adjecency matrix allows for both direction and weighting of networks, as shown in figure 2.2. When the Adjecency matrix is weighted, we use the letter W to describe it. Another helpful concept used for characterizing networks is the degree vector, $K(k_1, k_2, ..., k_i)$, of the nodes. The degree is the number of outgoing links from a given node and is given by summing the corresponding column of the matrix,

$$k_i = \sum_j A_{ij}.$$

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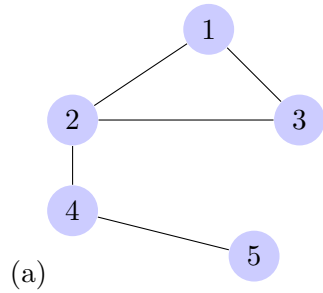
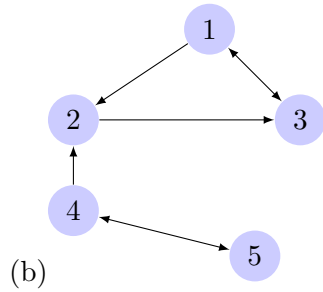


(a)

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

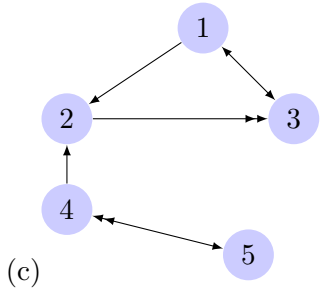
$$K = [2, 3, 2, 2, 1]$$



(b)

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$K = [2, 1, 1, 2, 1]$$



(c)

$$W = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$K = [2, 2, 1, 1, 2]$$

Figure 2.2: The figures represents different networks and their corresponding Adjecency matrices, A, and degree vectors, K. Subfigure (a) shows an undirected, unweighted network. The corresponding Adjecency matrix is symmetrical and consists only of zeros and ones. Subfigure (b) shows a directed, unweighted network. The Adjecency matrix is not symmetrical and consists only of zeros and ones. Subfigure (c) shows a directed, weighted network. The weighted Adjecency matrix is not symmetrical, and consists of values zeros, ones and twos. In principal, all real numbers can be chosen for the weights, but integers was chosen for a better visual illustration.

2.2.5 Dynamic Networks

The idea of a dynamic network is essentially to construct a network with nodes and edges, place a number of walker particles on the network, give the walkers rules of dispersion, and let the system propagate in time. The model can represent a variety of real-world phenomena, such as disease spreading, both in the microscale between cells and macroscale between cities, car traffic modelling, power grid networks, and generally all types of networks that has a traffic of information between its nodes. In later years, some work has focused on determining topographical features of networks by allowing walkers to spread across networks and mapping the time-development. In 2005, Simonsen wrote a summary of the results he had come to by allowing diffusion processes to take place on a network[15]. Just by observing the dispersion of walkers, attributes like clustering (or as it is described in the paper, modularity), were measured. The process has also been used by Newman [16], to simulate spreading of deseases and computer viruses on networks, giving information about how the systems topography can decide whether a certain epedemic will continue to spread to the whole network or simply vanish. Both the papers by Simonsen and Newman give an extensive introduction and summary of the science done in the field so far, and is worth to read for further explanations. They have both been used as a reference when writing this chapter.

2.2.6 Diffusion on Networks

Different rules of dispersion can lead to very different time propagations. In this thesis a simple diffusion model has been used, following Einsteins description of brownian particles[17]. These particles behave completely random, and their movement will have the same probability for moving in any available direction. Adapted to our network, the model sets the rule to be that a particle at one node will with move to one of the nodes it is linked to with the same probability if the system is un-weighted, and with a probability proportional to the weight of the link if weighted. The choice has also been made that all the particles present on node j at time t will move away from it when the system propagates in time to $t + 1$.

In order to not have to simulate each of the particles' random outcome, the number of particles is very much larger than the number of nodes $n \gg N$. The number of particles going from node $j \to i$ at time t, $C_{ij}(t)$ per weight unit, will then be completely determinalistically decided by the population on the node, $\rho_j(t)$, the degree of the node, k_j, by the formula

$$C_{ij}(t) = \frac{\rho_j(t)}{k_j}. \tag{2.5}$$

This traffic gives in time the master equation for determining the time development of node population,

$$\rho_i(t+1) = \sum_j W_{ij} \cdot \frac{\rho_j(t)}{k_j}. \tag{2.6}$$

Chapter 3

Network Entropy

Some work has been done on entropy of complex networks, but so far the focus has been on an entropy defined by the network itself. For instance, Robert Ash already in 1965 in his book "Information Theory" defined an entropy of networks as a measure of how uniform it was, i.e. how much you could know about any distinct node, by knowing about the whole network[18]. A uniform degree distribution would for instance give a lower entropy than a network with vastly different degrees over the nodes. Instead of focusing on the entropy of the network topology, a different approach would be to define an entropy for the information flow in the system.

3.1 Dynamical Network Entopy

The main goal of this thesis is to define the quantity entropy in the field of dynamic networks. In order to define the new term, a few conditions has to be set. First of all, the entropy has to be computable at any instant of an ongoing network simulation to allow for the study of its time development. Secondly, as we are dealing with systems with a time dimension, the variable should for unperturbed systems always increase monotonically towards an end value, where the entropy is maximized, as

dictated by the second law of thermodynamics.

To fulfill these conditions, the entropy of a dynamic network per walker is chosen to be defined as the sum of the traffic of walkers on the links connecting the nodes together, times the weight of each link in the familiar $p\ln(p)$ formula used by Shannon, equation2.4,

$$\frac{S(t)}{n} = -\sum_{ij} W_{ij} \frac{C_{ij}(t)}{\sum_{nm} C_{nm}(t)} \ln\left(\frac{C_{ij}(t)}{\sum_{nm} C_{nm}(t)}\right), \tag{3.1}$$

where n is the total amount of walkers in the system defined by adjecency matrix, W_{ij}, and C_{ij} is the amount of walkers travelling on the link between node i and j in direction $j \to i$.

The choice to define the entropy in a "per walker" fashion, comes directly from the thermodynamical equivalence, that has a higher entropy for a higher number of particles. If not for the "per walker"-definition, the system would have had the same entropy for any number of walkers. An interesting feature with this variable, is that its time development is a function of variables coming from both the rules of the dispersion of walker particles, and also topographical features of the network itself. The time development of the entropy will vary significantly for different networks, and also for different dispersion rules.

For the unconstrained state, the amount of walkers going from node i to j in timestep t, will be given by (2.5).

An important thing to note is that this definition has the p=value from 2.4, defined in such a manner that the entropy from a 2-weighted link is the sum of two 1-weighted links, as opposed to calculating it with the adjecency matrix element also being a factor inside the paranthesis. This was a matter of definition, and by choosing in this matter it was possible to trivially calculate a stationary state entropy, a very useful value for analyzing the results. In the case of Brownian walker diffusion, a stationary state is reached at $t \to \infty$ and the amount of walkers at each node i will then be given by

$$\rho_i^{\infty} = n\frac{k_i}{\sum_i k_i}, \tag{3.2}$$

where n is the total amount of walkers populating the entire system. This expression is found trivially by concidering that in an equilibium state, every node has ah same weight on links leaving the node as coming in in each time step, and thus the population on each node must be proportional to its total relative weight. By inserting this into equation (2.5), the term for the traffic per weight unit on link ji in an unconstrained network at $t \to \infty$ is

$$C_{ij}^{\infty} = \frac{n}{\sum\limits_j k_j},$$

with

$$\sum_{ij} C_{ij} \cdot W_{ij} = n.$$

Inserting these expressions into the equation (3.1), the entropy, S, at $t \to \infty$ for a network without constraints is given by

$$S^{\infty} = -\sum_{ij} W_{ij} \frac{1}{\sum\limits_{nm} W_{nm}} \ln\left(\frac{1}{\sum\limits_{nm} W_{nm}}\right).$$

If one defines $L = \sum_{ij} W_{ij} = \sum_j k_j$,

$$\begin{aligned} \frac{S^{\infty}}{n} &= -\sum_{ij} \frac{W_{ij}}{L} \ln\left(\frac{1}{L}\right), \\ &= -L\frac{1}{L} \ln\left(\frac{1}{L}\right), \\ &= \ln L. \end{aligned} \tag{3.3}$$

From thermodynamics, it is expected that when adding two systems with entropies A and B, the resulting equilibrium entropy per particle should be larger than for the two systems on their own, due to the increase in number of spaces each particle is able to occupy,

$$S_{AB}^{\infty} > S_{A}^{\infty} + S_{B}^{\infty}. \tag{3.4}$$

This is also the case for the defined entropy for networks, by equation (3.3), as

$$n_B \ln(L_A) + n_B \ln(L_B) > (n_A + n_B) \ln(L_{A+B}),$$

because of the nature of the logarithm, which states

$$\ln(x) > \ln(y) \quad \text{if } x > y.$$

Chapter 4

Evaluation of the Dynamic Network Entropy

4.1 Method

4.1.1 Networks

In order to simulate the time development of network systems, different kinds of networks was used.

The Karate Club Network

A well known real-world example of a network is known as the *karate club network*. The network originates from sociologist Wayne Zacharys studies of the social network in a karate club at an American university in the 1970s[19]. During the studies, the club went through a turbulent period over economical issues and broke up into two fractions, one with supporters of the trainer and one with supporters of the administrator. Figure 4.1.1 shows the layout of the network, including the division into two fractions. The karate network is in its original form weighted by integers 1-7, representing how strong the relationship between two people

was, and both this original form, and an unweighted version of it, i.e all weights equal to one, will be considered.

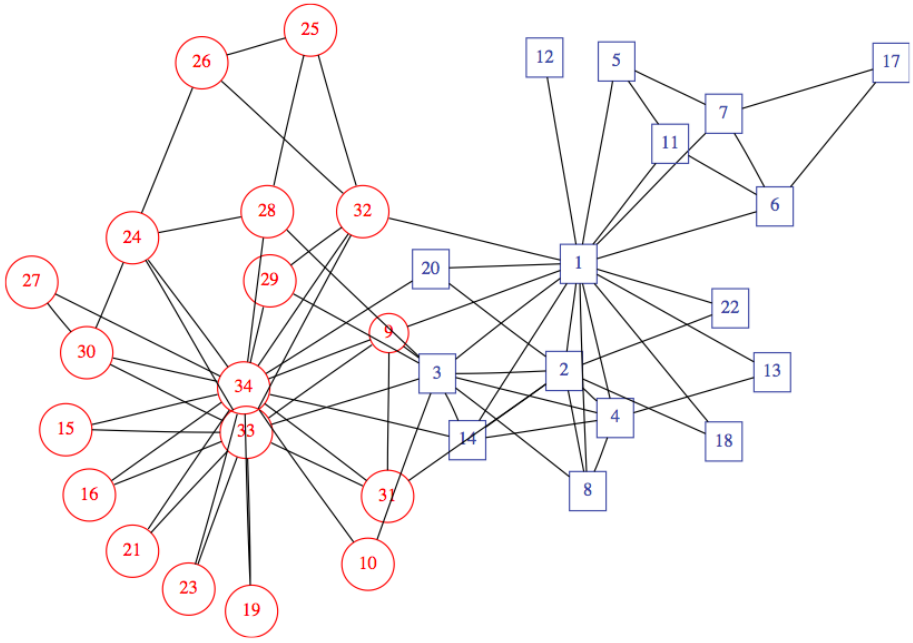


Figure 4.1: The figure shows Zacharys karate network with unweighted, undirected links. Squares and circles are used to represent membership in a subgroup, resulting from the ongoing conflict, of the supporters of the trainer (node 1) and administrator (node 34). Figure taken from [15].

The Square Lattice Network

The square lattice network is essentialy an nxm matrix where all nodes are connected to four neighbours, one on each of its four sides.. The squarelattice can have different borderconditions, allowing for different shapes. The one used in this thesis is one where the opposite edges are connected to each other, so that the network represents a torus shape. This configuration is illustrated in figure 4.1.1. The squarelattice can have any size mxn. The algorithm for constructing this is

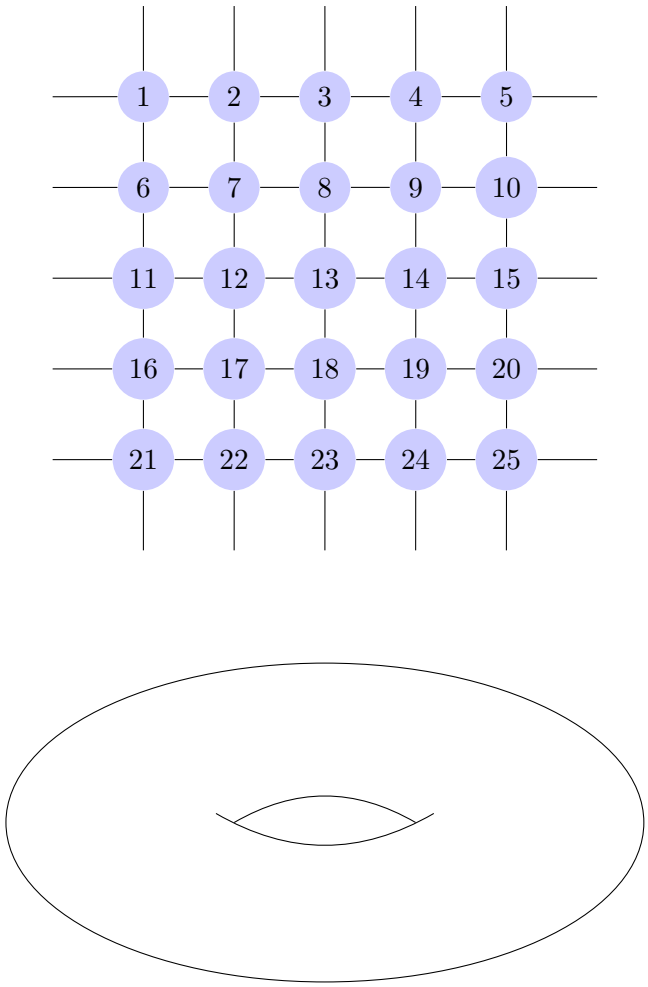


Figure 4.2: A square lattice with continious border conditions. each node is connected to four other nodes by an undirected link. The nodes on the edges are connected to the node on the opposite edge, thereby creating a torus topology.

Algorithms

The simulations were performed in Matlab, the R2011b edition, and all functions used in the algorithms are standard functions of Matlab. An algorithm was constructed in order to simulate the time development of the node populations in a network, and at the same time calculate the entropy, as defined in (3.1). The algorithm for the case where the nodes and links are unrestricted, is given by the scheme in algorithm 1.

Algorithm 1 Translate $\rho(t)$ from $t \to t+1$ and get entropy

```
Given vector ρ(t), containing node populations, Adjacency matrix, W,
number of walkers, n
K=sum(W)
entropy=0
for i=1:length(W) do
  for j=1:length(W) do
    newρ(i)=newρ(i)+A(i,j)·ρ(j)/K(j)
    tmpS=W(i,j)*ρ(j)/K(j)/n·log(W(i,j)·ρ(j)/K(j)/n)
    if tmpS==NaN then
      tmpS=0
    end if
    entropy=entropy+tmpS
  end for
end for
N=newN
```

The K vector represents the number of outgoing links per node. The temporary S value is simply there to make sure that the entropy will not contain NaN values in the cases where the argument of the logarithm is 0. The analytical value for these terms are

$$\lim_{x \to 0} x \log x = 0,$$

so the numerical method has to be corrected for.

In some cases, there is an interest in connecting two networks to each other. In Matlab, this is a simple task to perform, and the method is given in algorithm 2.

Algorithm 2 Connecting two networks represented by Adjecency matrices A and B, into new network C at nodes N_A and N_B by weights w_{AB} and w_{BA}

C=zeros(length(A)+length(B))
C(1:length(A),1:length(A))=A
C(length(A)+1:length(C),length(A)+1:length(C))=B
C(N_A, N_B)=w_{AB}
C(N_B, N_A)=w_{BA}

4.2 Results

Simulations using Algorithm 1 to transfer in time enables the plotting of the entropy S, as a function of time. All systems considered have a start configuration with an initial distribution of all the walkers on a given node, giving the lowest possible entropy to start with.

4.2.1 Entropy Development on Undirected Networks

The Karate network

The entropy developements on the karate club network shows a satisfying progression, increasing monotonically towards the analytical result for the equilibrium state entropy in accordance with the behaviour predicted by the second law of thermodynamics. The theoretical equilibrium entropy is higher for the directed one, which is expected as the average number of unit weight per link is higher. As the system entropy reaches the theoretical value, calculated from (3.3), the distribution of node population proportional to the degree of the link is reached, in accordance with the predictions given by equation (3.2).

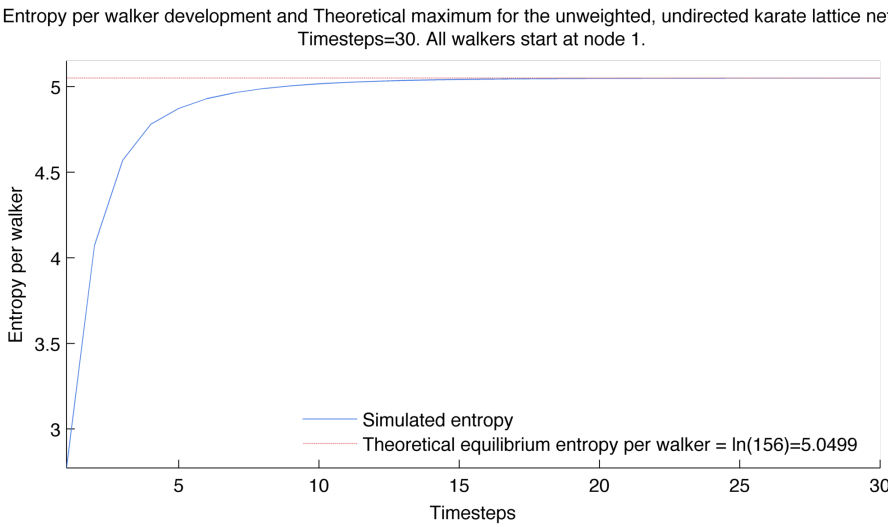


Figure 4.3: Entropy development in the unweighted, undirectional karate network. The theoretical equilibrium entropy is calculated from equation (3.3).

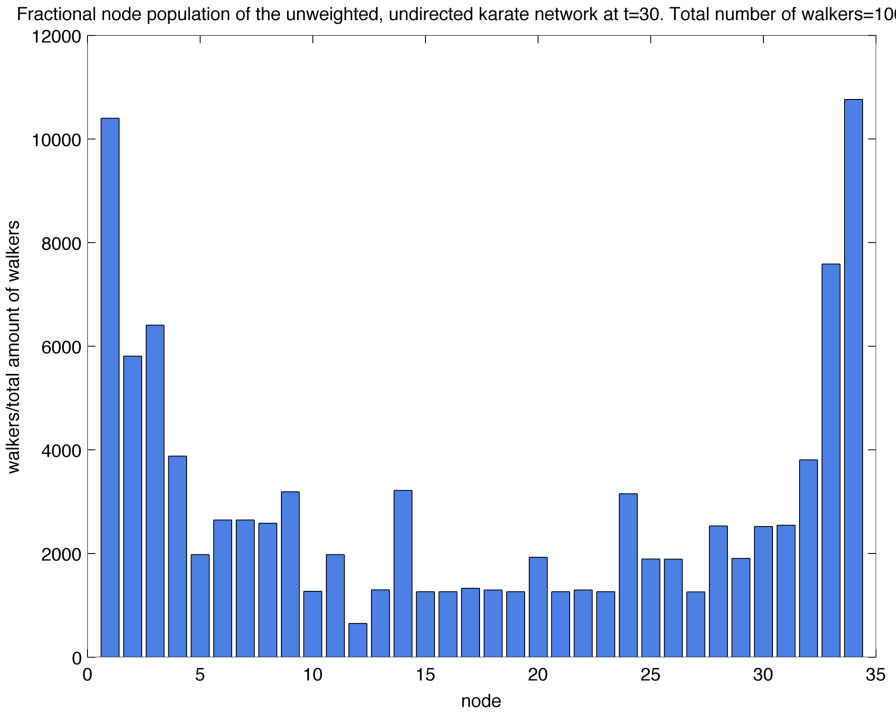


Figure 4.4: Node distribution of the unweighted, undirectional karate network. The distribution is the corresponding to the theoretical given by equation (3.2).

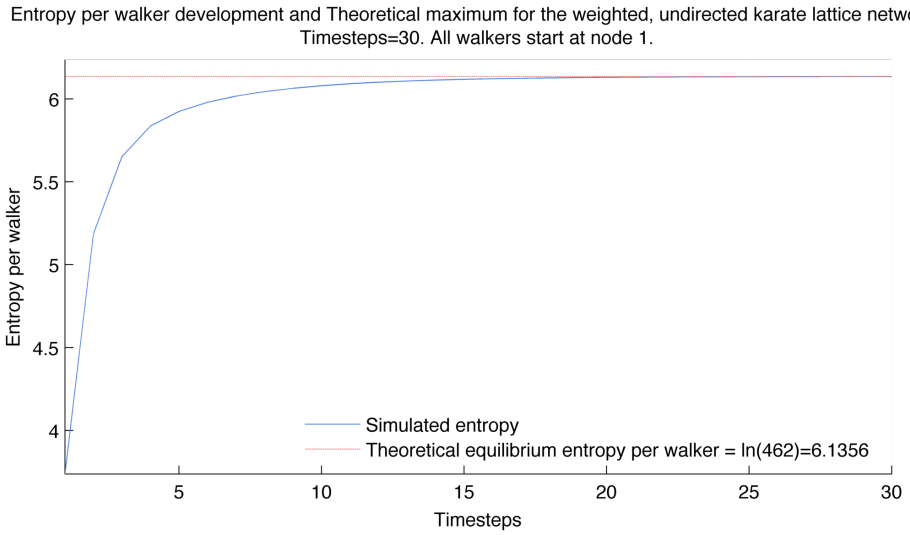


Figure 4.5: Entropy development in the weighted, undirectional karate network. The theoretical equilibrium entropy is calculated from (3.3),

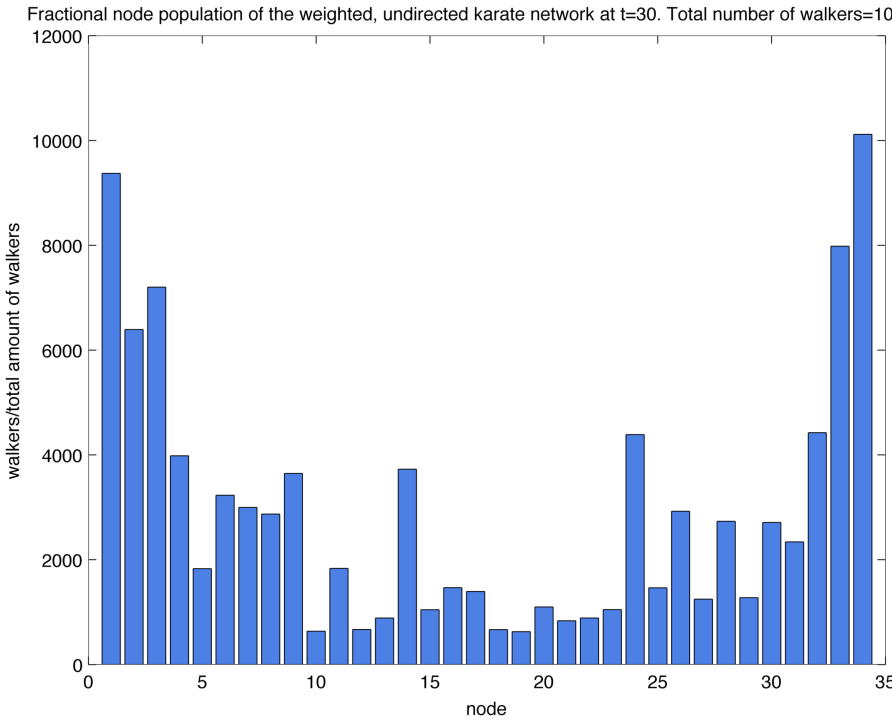


Figure 4.6: Node distribution of the weighted, undirectional karate network. The distribution is the corresponding theoretical from (3.2).

The Square Lattice network

For the 15×15 square lattice network, the entropy progresses the expected way, as was the case for the karate network. The weighted network behaves in a similar manner, but is not included here as it is considered to not provide any additional information.

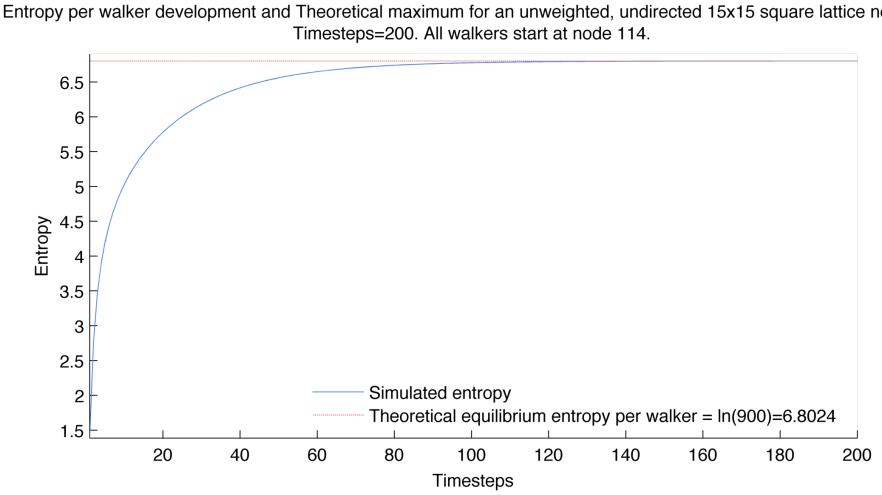


Figure 4.7: Entropy development of the unweighted, undirectional15×15 square lattice network. The theoretical equilibrium entropy is calculated from (3.3).

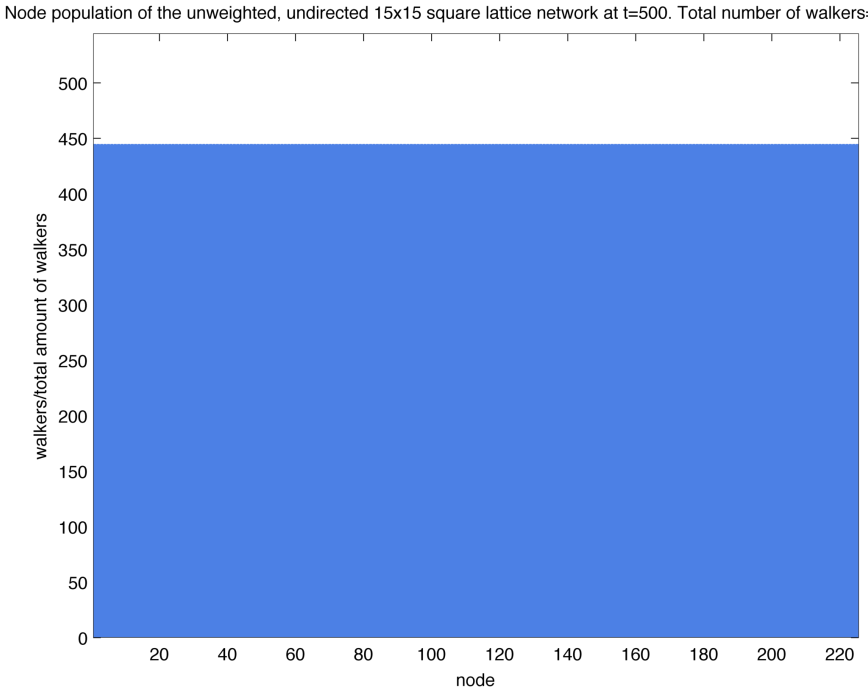


Figure 4.8: Node distribution of the unweighted, undirectional 15×15 network. The final distribution is even across all nodes, corresponding to the theoretical calculated from from (3.2).

In square lattice networks, there is an issue for $n \times n$ lattices when n is an even number. A closer look at the distribution shows that even numbers causes the walkers to only occupy the half of the nodes at each timestep like in a chess board. The nodes that are occupied changes every timestep as can be seen in 4.2.1. This prevents the system of reaching its theoretical maximum entropy. Square lattices with n being an even number, will therefore not be used for the remainder of this thesis. One could, however, circumvent the problem by redifining the theoretical entropy from (3.2) to only sum over links with traffic.

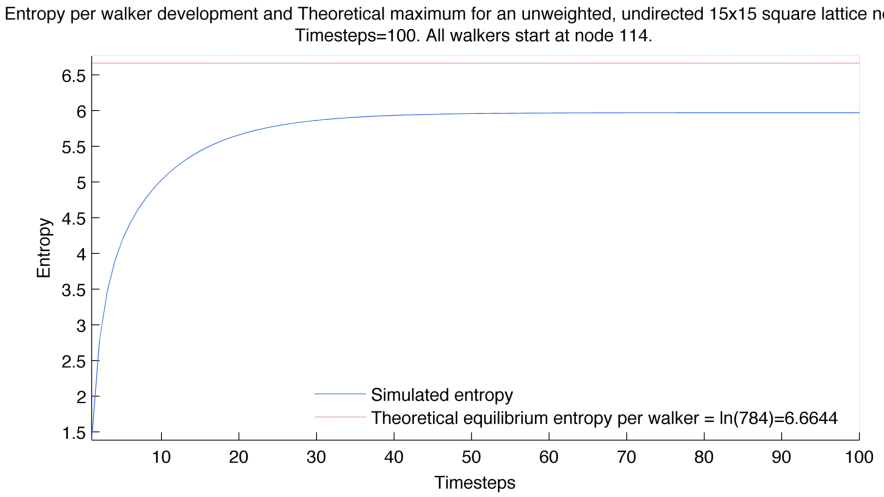


Figure 4.9: Entropy development of the unweighted, undirectional 14×14 square lattice network. The theoretical equilibrium entropy is calculated from (3.3).

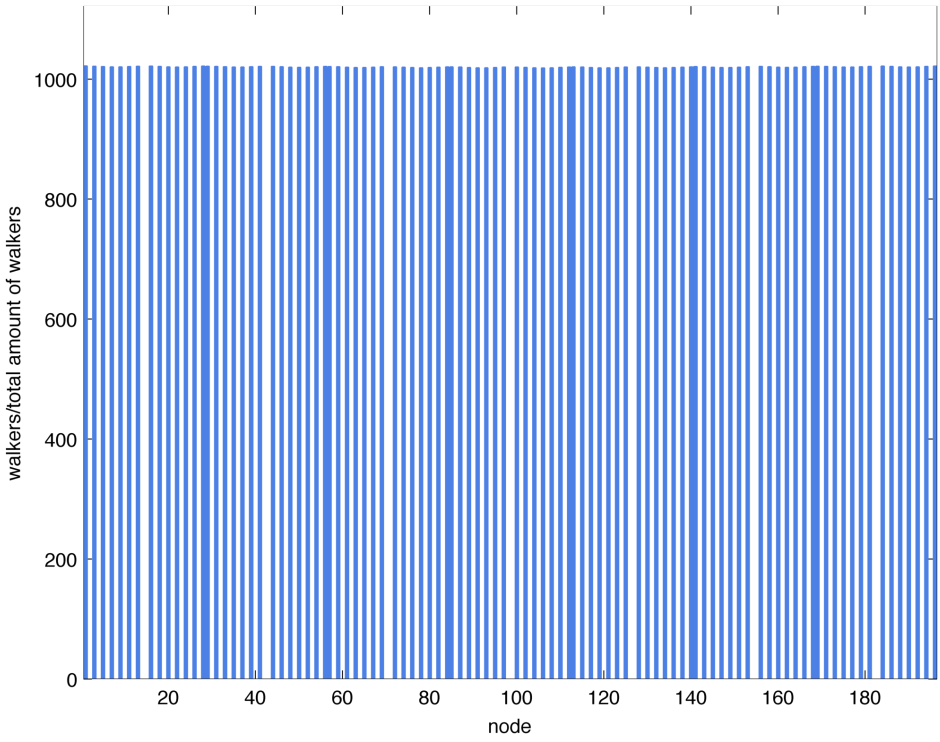


Figure 4.10: Node distribution of the unweighted, undirectional 14×14 square lattice network. The final distribution is not the corresponding to the theoretical from (3.2), but rather every other node is occupied/unoccupied.

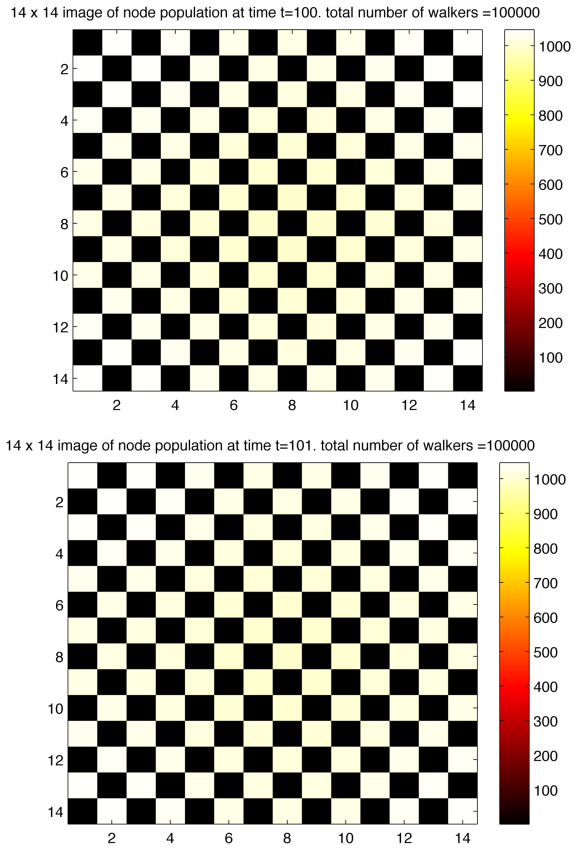


Figure 4.11: Illustration of the interchanging chess board behaviour of an even number square lattice at two times t and $t+1$. The picture represents a 14×14 lattice, where each square represents a node, node 1 being at the upper left corner, and node 2 to the right of it. Notice that node 1 is black at one time, and white in the second, which represents that the node is empty and populated, respectively. The color of the nodes is representing the popilation on each node by the scale provided in the figure.

4.2.2 Directed Networks

The networks can, as discussed in theory, be directed with an unsymmetric Adjecency Matrix. In this section, the weighted karate network will be used, with some modifications to make it directed. One interesting thing with directed networks is that they introduce a constraint on the flow of particles. These constraints can in turn lead to congestions in the network, with more particles in one area than others. In the following, the modifications that are done are done with the purpose of showing these effects.

First, a modification is made on the karate network where one removes the link going from node $3 \rightarrow 1$, and from node $1 \rightarrow 9$. This does not congest the system at all, as the walkers on one of these nodes, can reach the walkers on the other node in the pair by going through other nodes. The calculated equilibrium state entropy will change slightly from the original network as links are removed, but it is still defined in the same way. As shown in figures 4.12 and 4.13, the entropy behaves as for the undirected networks, and reaches the equilibrium entropy and distribution.

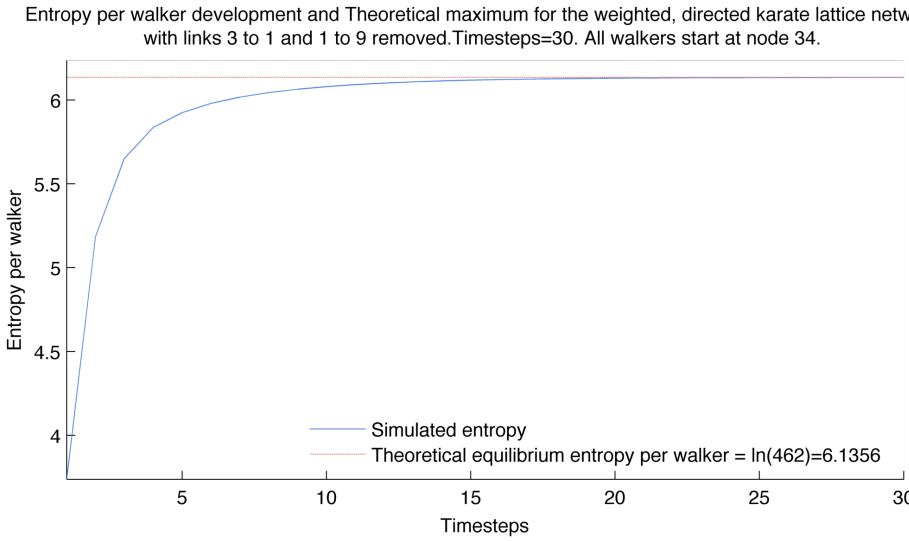


Figure 4.12: Entropy development in the weighted, directed karate network with no congestion. The theoretical equilibrium entropy is calculated from (3.3),

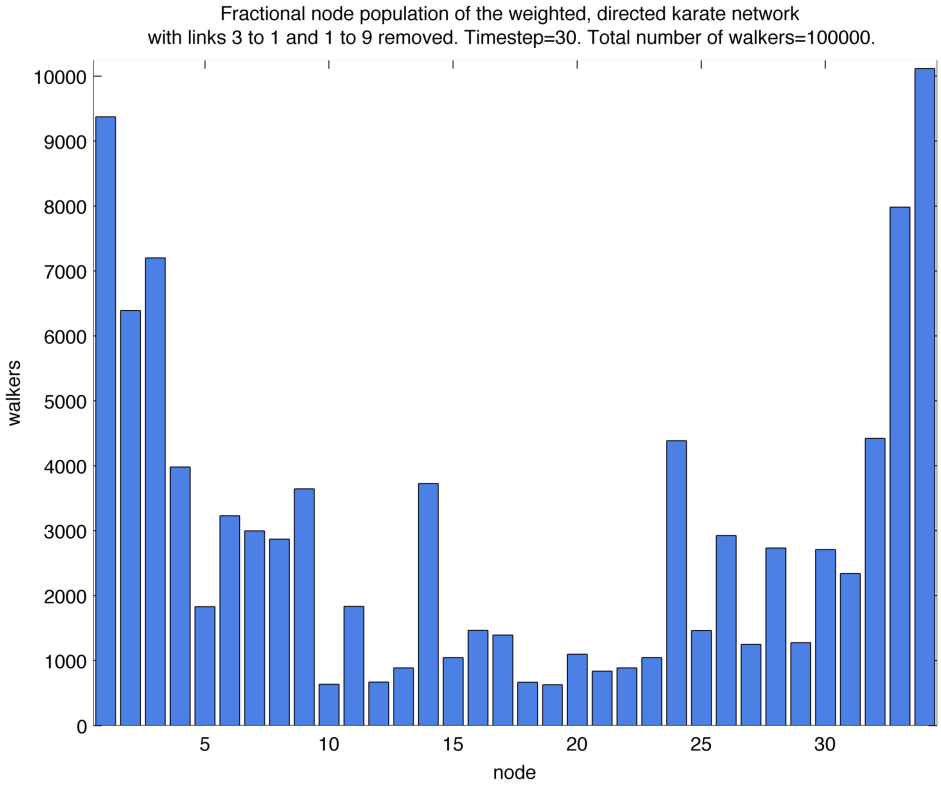


Figure 4.13: Node distribution of the weighted, directed karate network with no congestion. The distribution is the corresponding theoretical from (3.2).

To demonstrate the extreme case of congestion, the modification done on the weighted karate network is the removal of the links $5, 6, 7, 11 \rightarrow 1$. This leads to all the walkers accumulating at the nodes in the upper right corner of figure 4.1.1. The results shown in figures 4.14 and 4.2.2, show how the entropy at first increases as the walkers are dispersed over the whole network at first, but then decreases towards stability as the walkers get accumulated on nodes 5, 6, 7 and 17.

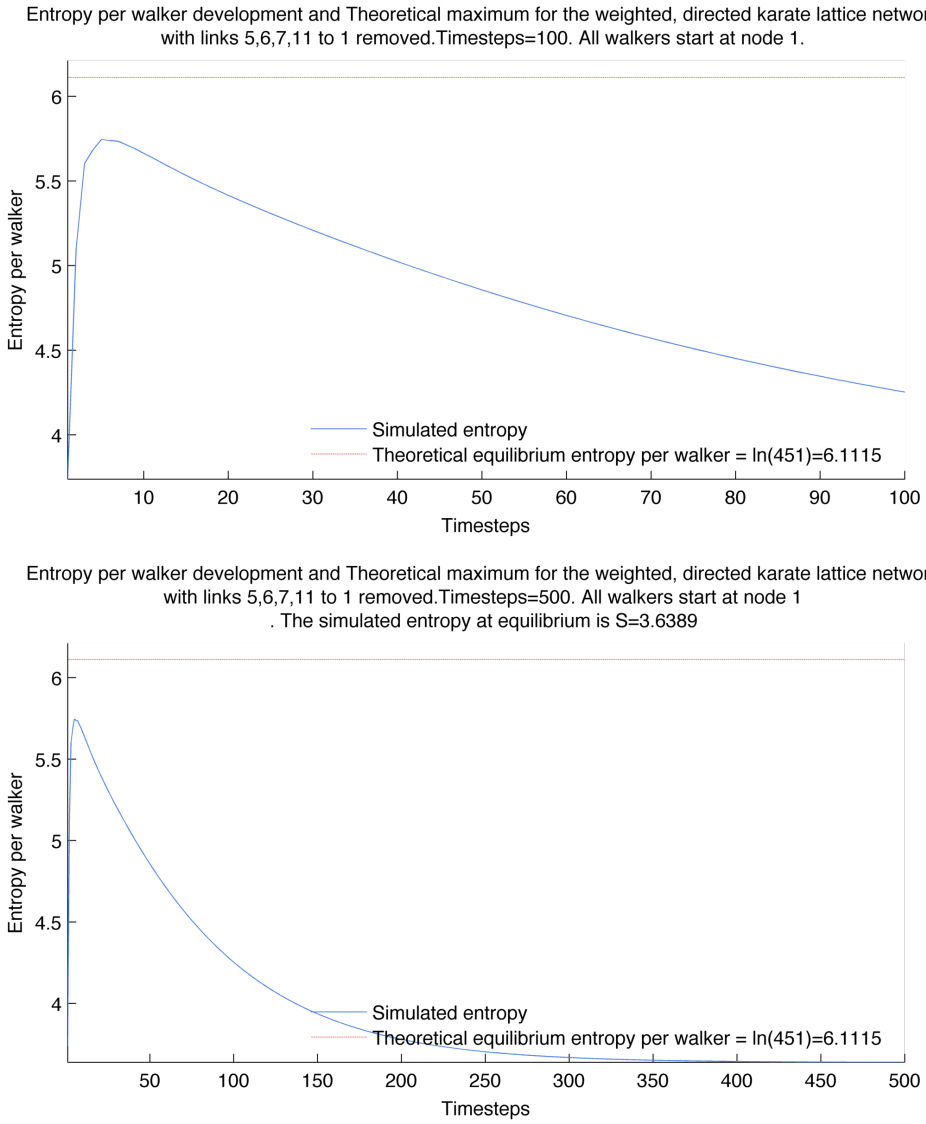


Figure 4.14: Entropy development in the weighted, directed karate network with full congestion shown in two plots with different axes. The theoretical equilibrium entropy is calculated from (3.3),

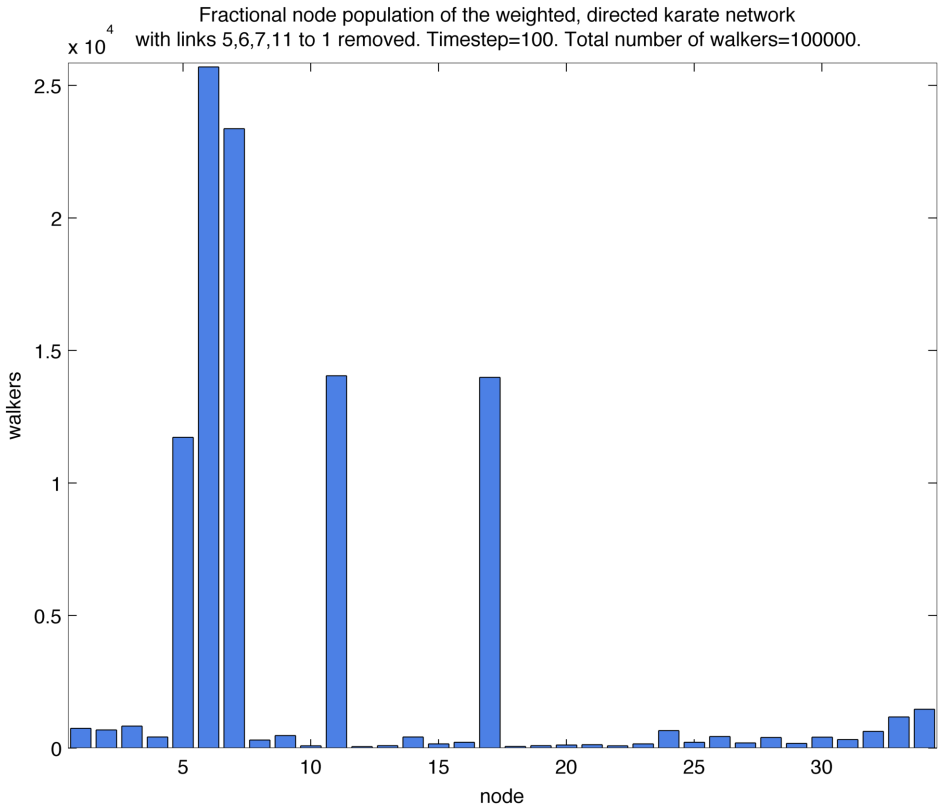


Figure 4.15: Node distribution of the weighted, directed karate network with full congestion, having most of the walkers concentrated on nodes 5, 6, 7, 11 and 17.

In addition to the two extreme cases of no congestion and full congestion, there is a case in between. Instead of removing the links $5, 6, 7, 11 \rightarrow 1$, their weight can be set to a low value, say 0.25. For this configuration, there will be a partial congestion on the subgroup of nodes 5, 6, 7, 11 ,17, but, the equilibrium still has walker population on the rest of the nodes, as shown in figures 4.16 and 4.2.2.

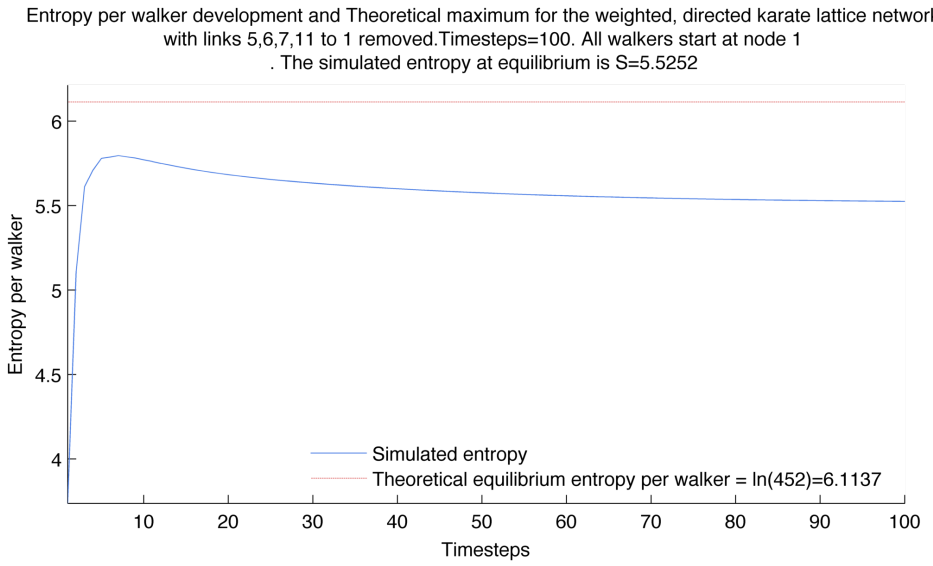


Figure 4.16: Entropy development in the weighted, directed karate network with partial congestion. The theoretical equilibrium entropy is calculated from (3.3).

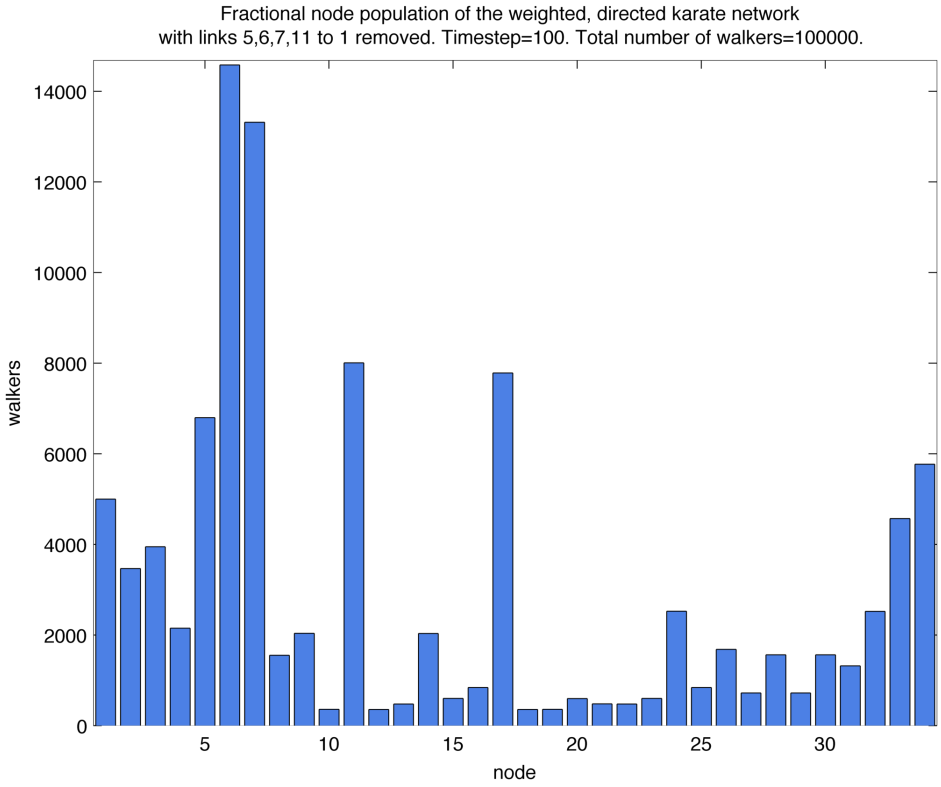


Figure 4.17: Node distribution of the weighted, directed karate network with partial congestion.

A suggestion as to how one should quantify the congestion of a network would be to compute the relation between the between the simulated and theoretical equillibrium state entropy,

$$\text{Congestion} = \frac{S_{\text{simulated}}}{S_{\text{theoretical}}}.$$

This number would be ranging from 0 to 1, where 0 indicates the case where all the walkers are at one node and there is no traffic on any link, and 1 indicates no congestion. The values for the three cases considered in this section is given in table 4.2.2. I

Network	$\boldsymbol{S}_{\textbf{simulated}}$	$\boldsymbol{S}_{\textbf{theoretical}}$	**Congestion**
No Congestion	6.1356	6.1356	1
Full Congestion	3.6389	6.1115	0.5954
Partial Congestion	5.5252	6.1137	0.9037

4.2.3 Mixing of Networks

Having two networks with an initial configuration of walkers on each of them, should lead to an equilibrium entropy larger for the resulting system than if the two systems were kept separate. The mixing is performed by at time= t_mix changing the adjecency matrix to include a link between two chosen nodes in network A and B, according to algorithm 2. The algorithm gives $L_{AB} = L_A + L_B + 2$

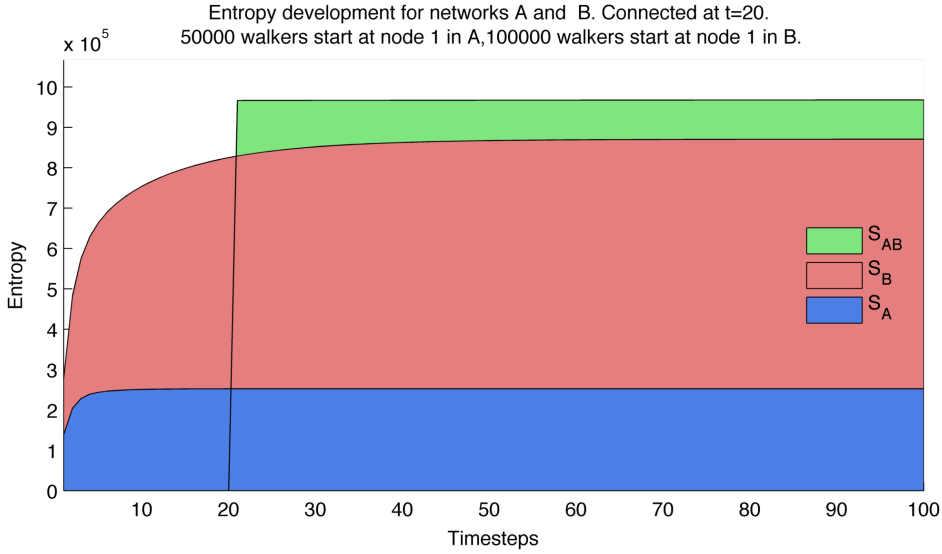


Figure 4.18: Entropies for the unweighted, undirected karate network (A) and an unweighted 11x11 square lattice network (B) connected together at time t with a link between node 1 in A and B, with weight 1 in both directions. The connection is indicated by the vertical black line. The blue and red areas shows the entropies for A and the B respectively. To the right of the black line, the areas show the entropy of A and B as they would have developed without connection. The green area shows the extra contribution from the connection between the two networks.

The entropy after mixing of two networks behaves as expected from equation (3.4), with

$$\begin{aligned} S_A^\infty &= n_A \cdot \ln(L_A) = 50000 \cdot \ln(156) = 2.5249 \cdot 10^5, \\ S_B^\infty &= n_B \cdot \ln(L_B) = 100000 \cdot \ln(484) = 6.1821 \cdot 10^5, \\ S_{AB}^\infty &= (n_A + n_B) \cdot \ln(L_A + L_B + 2) = 150000 \cdot \ln(642) = 9.6969 \cdot 10^5. \end{aligned}$$

These results shows how the suggested entropy fulfills yet another property commonly associated with the thermodynamic property.

Chapter 5

Applications

The suggested dynamical entropy has so far satisfied the properties expected from its thermodynamic analogue, and it is therefore useful to show some applications of the variable. Some applications of the variable follows here.

5.1 Determining Node Centrality by Use of Start Node Variation

The information of which nodes in a network that are the most important cab be concidered by looking at what we define as node centrality. This attribute is very interesting in many cases. For instance, if the network models a car traffic network, with links as roads and nodes as intersections. In this case the most central node will be the intersection with most traffic on it, and thus the intersection most probable to be congested. If the network models the internet, the most central nodes are the servers most vital to keeping the internet online, and should therefore be more protected against hacker attacks. In general, the centrality of the nodes is valuable information about how important each node is to sustaining the information flow through the network.

5.1.1 Method

The method is based on the fact that the more central a node is, the faster the information from this node will disperse evenly over the network, i.e. reach S^{∞}, faster. For a demonstration of this property, see figure 5.1.1. Have all the walkers start at one node and log the entropy after a time T. For times $0 < T < T_{S^{\infty}}$, the entropy will increase towards S^{∞}. $T_{S^{\infty}}$ is the time when equilibrium is reached. The relative difference in values after the same time T chosen to be at a time where walkers are dispersed to all of the nodes, but for less than the lowest $T_{S^{\infty}}$ across all nodes, gives the relative centrality of the nodes. The method is given step by step in algorithm 3.

Algorithm 3 The variation of walker start node method, returning a entropy at time T for each of the nodes

```
Given a time, T, number of walkers, n, and the Adjecency matrix, W
entropies(1:length(W))=0
for i=1:length(W) do
  for t=1:T do
    Perform algorithm 1
  end for
  entropies(i)=entropy(T)
end for
N=newN
```

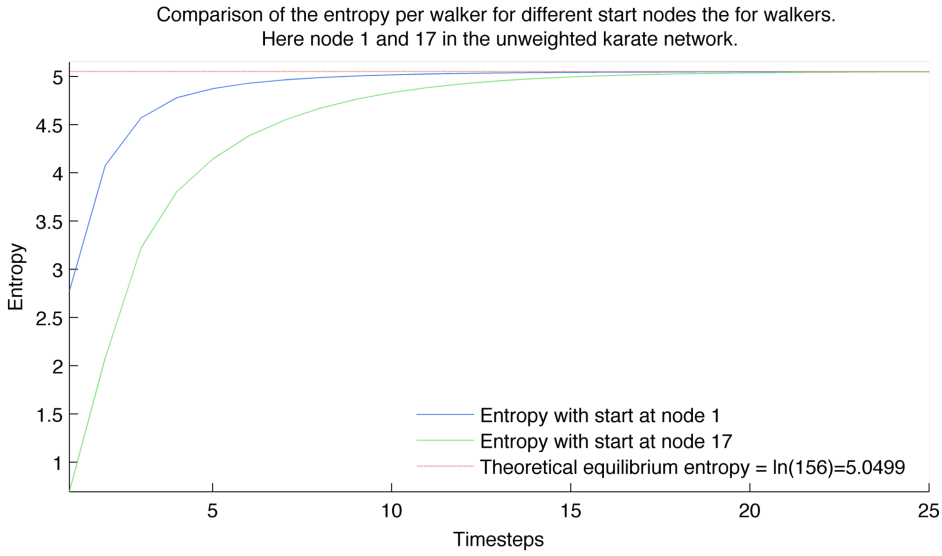


Figure 5.1: Comparison of entropy development for different cases of walker start distribution. Here, node 1 and 17 in the karate network are chosen, because from the illustration of the network, figure 4.1.1, node 1 is very central, and node 17 is located in the periphery of the network.

In order to show that the method works satisfactory, a centrality network is constructed. This network is a simple 7-node network, with node 4 being obviosly the most central. When the method is run on this network it should give a higher relative $S(T)$ value for 4 than for the other nodes

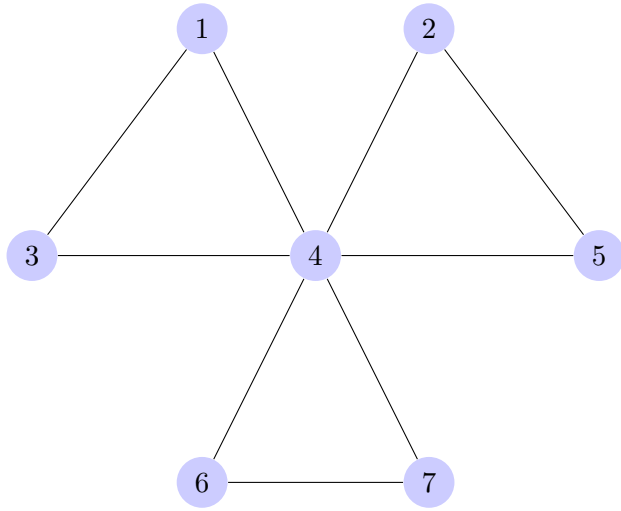


Figure 5.2: The centrality network is designed to have a node with a higher centrality than the others, here node 4.

5.1.2 Results

When performing the variation of start node algorithm on the constructed centrality network, it is evident that it behaves as expected. When all of the walkers started on thecentral node, the entropy had propagated closer to the maximum after $T = 3$ timesteps, than for the other more peripheral nodes, see figure 5.1.2. For all starting positions, the system would eventually move towards the same S_∞.

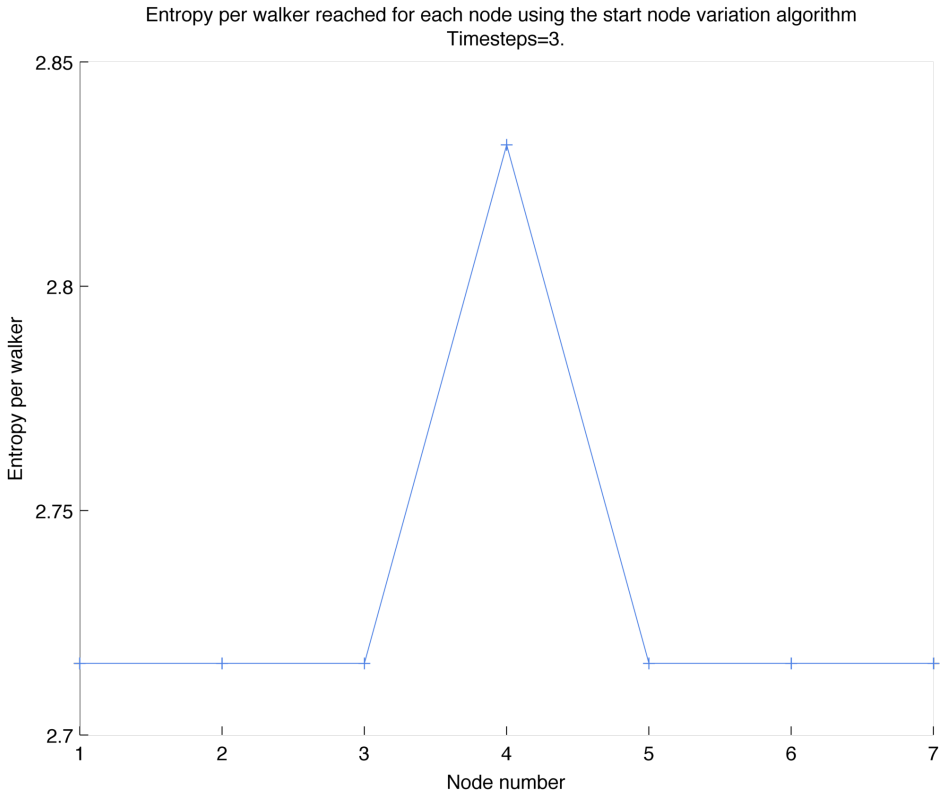


Figure 5.3: Entropies reached using the variaton of start node method on the centrality network after $T = 3$ timesteps.

The results of the variation of start node method on the centrality network was fairly easy to predict. For the unweighted karate network, it is not as trivial. If one consider the graphical representation in figure 4.1.1, one expects that the central nodes, such as node 9, 20 and 3 would be more central than the obviously peripheral nodes 12 and 17. For the rest, however, the results are not given.

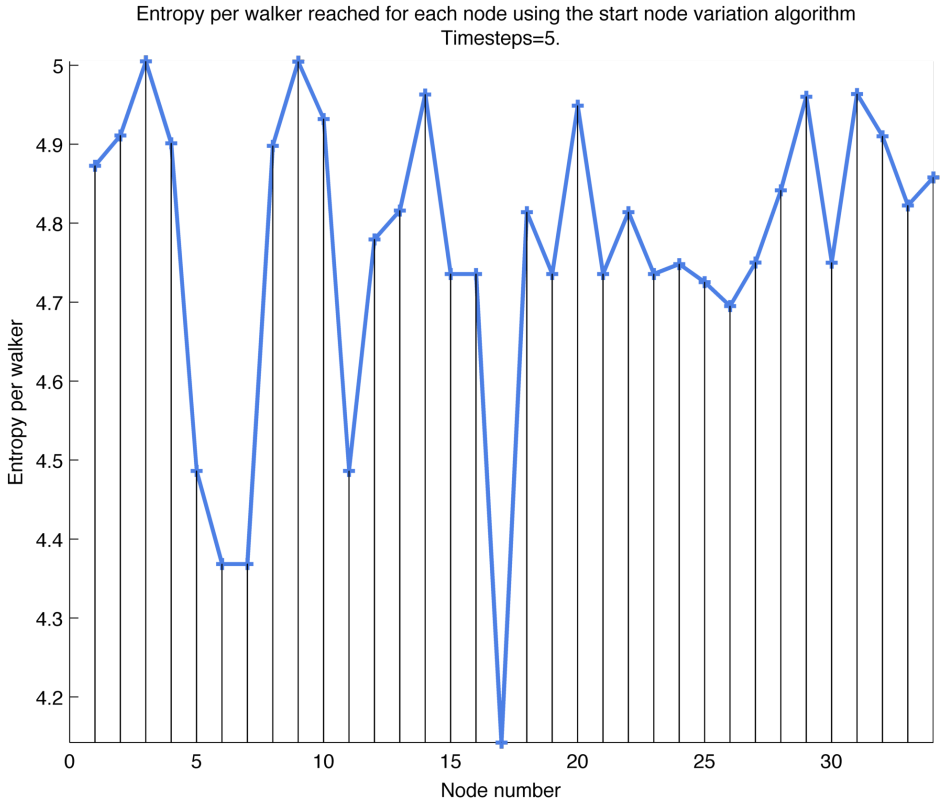


Figure 5.4: Entropies reached using the variaton of start node method on the unweighted karate network after $T = 5$ timesteps. Bars are added to make it easier to see which value represent each node.

In figure 5.1.2, the results are shown for performing the variation of start node method on the unweighted karate network. As expected, the most central nodes are nodes 3 and 9, with node 20 also having a high value. The least central node was node 17, which is also as expected. In addition to these points few interesting observations can be made as to how this method creates this hierarchy. From merely observing at the graphical representation of the network, one could easily assume that node 6 is more central, as it is linked to node 1 in the same manner as node 12, and also to additional nodes. Node 1 is important because it has a very high degree, 16, compared to the other nodes in the network. Getting walkers there is therefore very important to speed up the spreading of them, i.e augment the entropy. The reason node 12 is deemed more central than node 6 is that node 12 immediately sends all of its walkers to node 1, whereas node 6 disperses it equally between node 7, 17, 11 and 1.

As a confirmation, the method is also run on the uniform unweighted 15×15 square lattice network, and as expected, the distribution is completely uniform, as no nodes are more central than others, see figure 5.1.2.

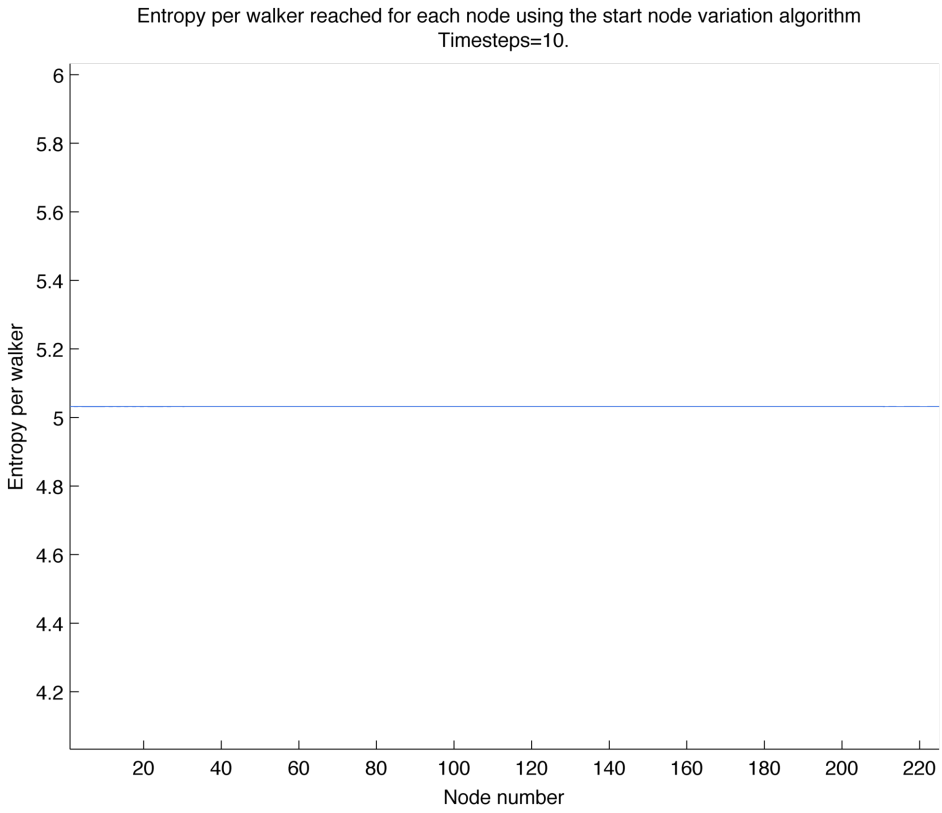


Figure 5.5: Entropies reached using the variaton of start node method on the 15×15 square lattice after $T = 5$ timesteps.

5.2 Mirror Network to Find Distances Between Nodes

In this section, the method of variation of start node will be used to create an hierarchy for the distance from one distinct node to the rest. This knowledge is valuable in the same way that centrality is valuable in order to understand the importance of nodes. It should be noted that the distance in question is not the geodesic distance, i.e the shortest possible distance, but the distance in terms of the time it takes to get information through the network from one node to another.

5.2.1 Method

The method is first a manipulation of the adjecency matrix in question, followed by the method of variation of start node. The method originally finds the most central node as the highest entropy after time T, and the others are hierarchally lower at the same time. The manipulation performed on the network in this method, is to copy the entire network into a mirror network, then combine the original network with the mirrored network at the node of interest. What is achieved by doing this is that the node of interest will become the most central node. The algorithm for this mirroring is shown in algorithm 4, and an illustration is given in figure 5.2.1.

Algorithm 4 The method of mirroring a network A, getting a new network C

Given an Adjecency matrix, A, and node of interest, x
B=A
combine matrices A and B by algorithm 2 into C
C(x, length(A)+x)=1
C(length(A)+x , x)=1

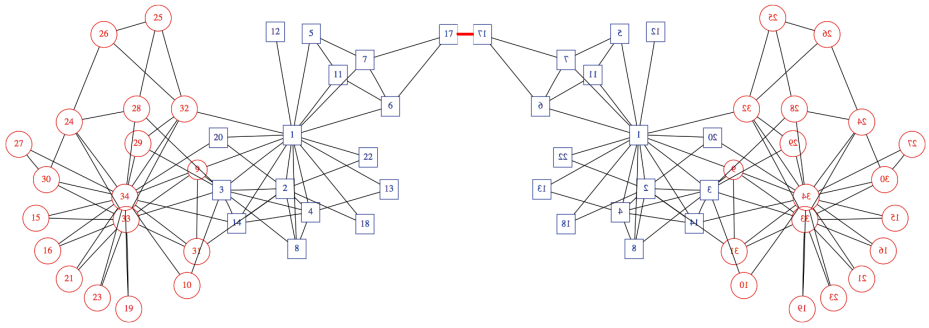


Figure 5.6: This is an illustration of the mirroring and connection to the mirror image of the karate network seen in figure 4.1.1. The red line shows the connection between the node of interest and its mirror node, here node 17. Mirror nodes are represented by their numbers being mirrored.

5.2.2 Results

In order to demonstrate the information given by this method, it is use to consider the 15×15 square lattice network. If on chooses the node of interest to be the center node, the distance from this node to the others should be larger the further from it one gets. This is certainly the case, and it is well demonstrated by the plot in figure 5.2.2 and even better by the 3D-plot of the same entropies in figure 5.2.2.

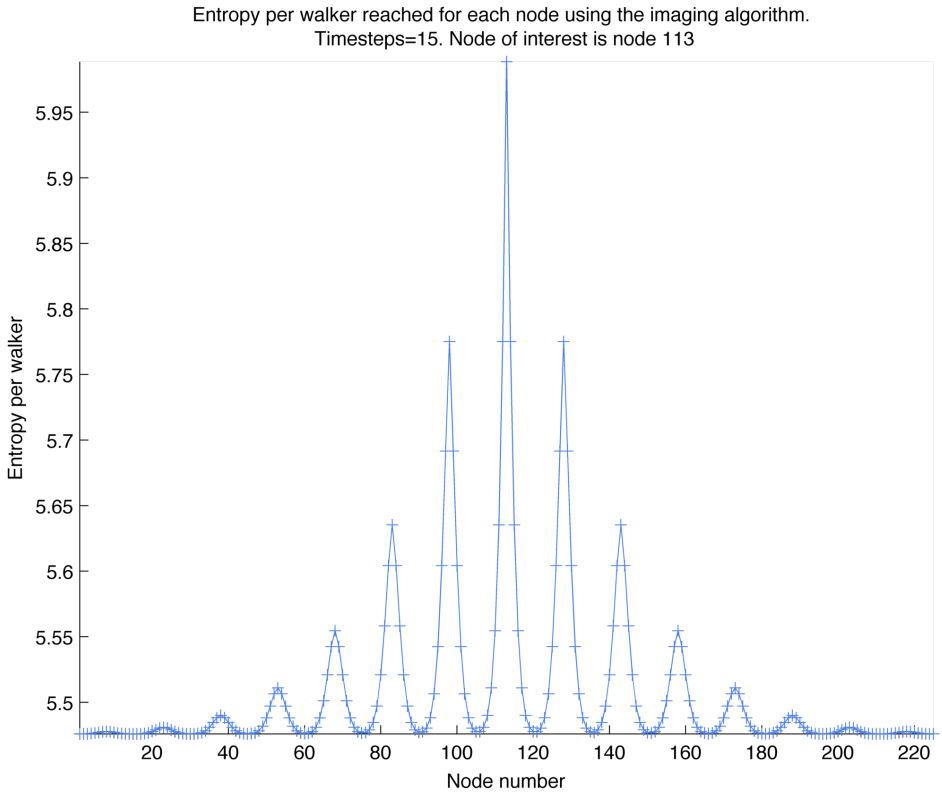


Figure 5.7: The mirror method performed on a 15×15 square lattice matrix.

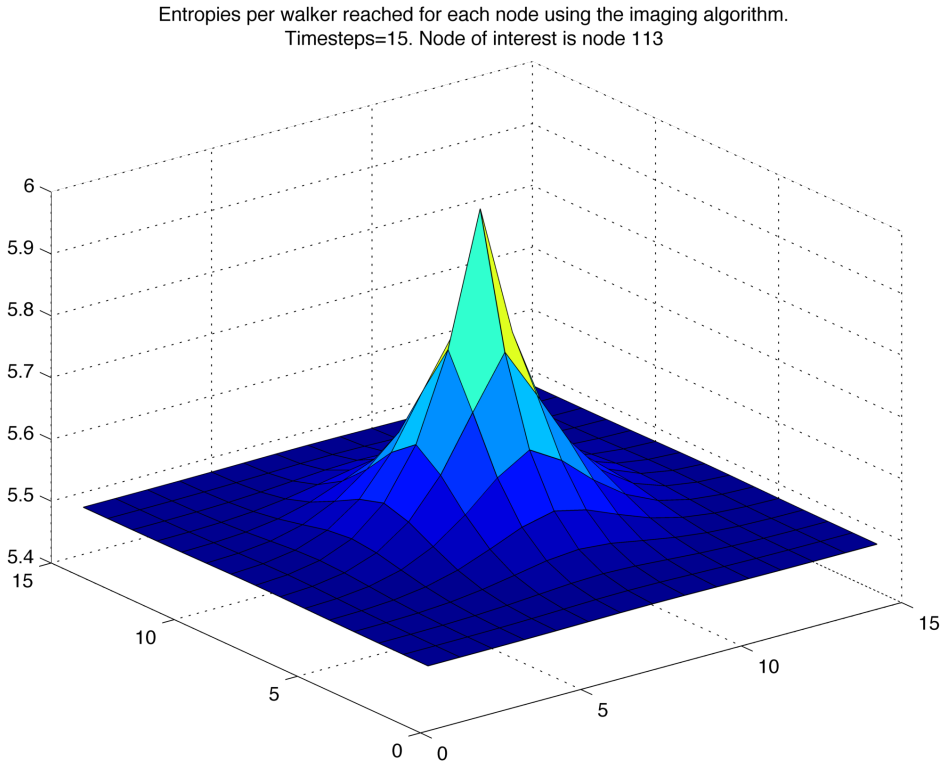


Figure 5.8: A 3D-representation of the imaging method performed on a 15×15 square lattice network. The node in the center of the surface is the node of interest. The square lattice is represented by the xy-plane, and the z-axis is the entropy.

The method was also performed on the unweighted karate network. Here it was chosen to use node 17 as the node of interest, so the mirroring would be of the form depicted in figure 5.2.1. From again observing figure 4.1.1, it was expected that nodes 7, 5 and 6 were the closest, and nodes on the other side of the figure, such as 27 and 15. These results were as expected, with low values for them both. Interestingly, the results shown in figure 5.2.2, indicated that the node with the longest distance from node 17 is node 28.

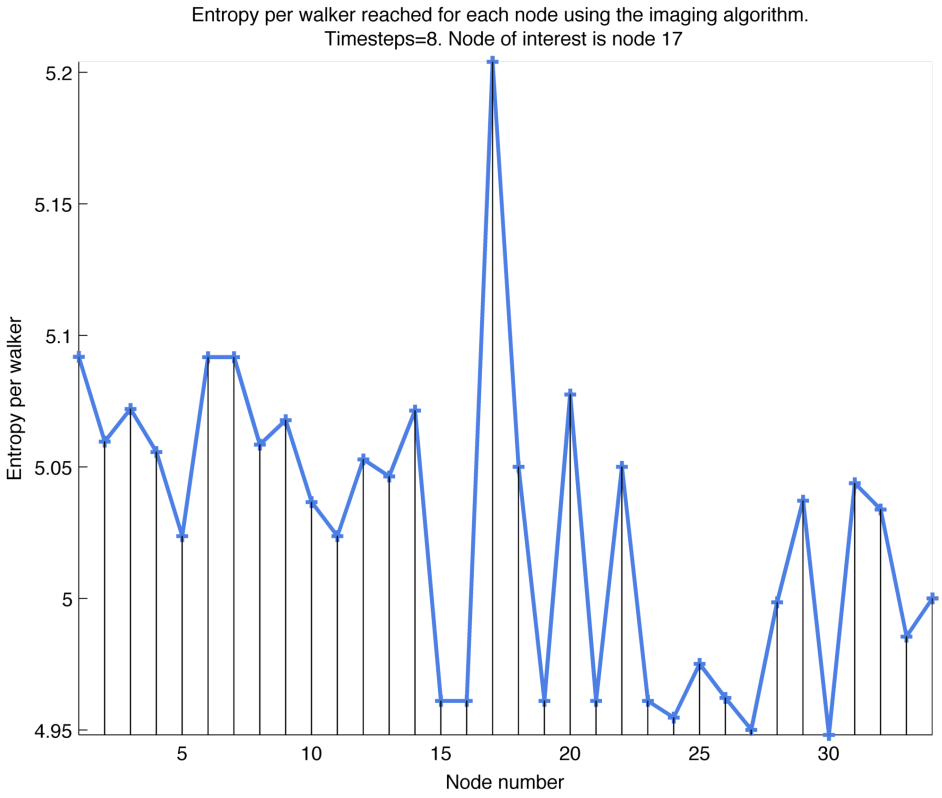


Figure 5.9: Entropies reached using the variaton of start node method on the karate network. Bars are added to make it easier to see which value represent each node.

This method measures the flow of information from the other nodes to the node of difference. This is distance is not necessarely the same in the other direction. Therefore, the method is limited in the way that one could only say in relative terms which nodes will be able to get information to the node in question, fastest and not the other way around.

Chapter 6

Conclusion and Further Work

6.1 Conclusion

In this thesis, a suggestion for a dynamical entropy as a function of walker traffic on the links between nodes in a network has been put forward. It was calculated for a diffusion process without constraints on various networks, and in these networks it behaved as expected when concidering the analogous variable in thermodynamics. The cases of directed systems where the theoretical value of equilibrium entropy was not reached do not break with the definition of the second law of thermodynamics. This is because the law is only expected to be valid for systems without constraints or perturbations, which directional links must be said to be.

The applications that were suggested were to some degree limited in their use, as they are just valid for the processes studied, and even under these terms, only relative values were given for centrality and information spreading distances. They are meant as suggestions for how one can go about to seek the meaning of the dynamical entropy in some networks, and should be considered under these terms.

6.2 Further Work

Regarding the further studies of the defined entropy, its behaviour should be examined for different processes on systems , as it is reasonable to expect that the entropy should be valid for any kind of processes on networks, though the processes should lead to a finite state dispersion of the particles in question for the value to have any practical importance. Types of networks that the entropy should hold for uncludes networks with sinks and sources, and limitations of node populations and link traffic. Networks that are developing in time are also natural to consider.

If one considers an real world car traffic network, and models it with a weighted adjacency matrix, the method of node variation could be used to explore whether frequently congested intersections corresponds to the most central nodes in the network. Assumingly, there have already been performed simulations of such problems, but it would be interesting to compare these results with the approach suggested in this thesis.

Models of desease spreading have been studied using diffusion processes earlier, and attacking the problem with an entropy approach could in some cases provide new knowledge. As the entropy is a function of both the processes taking place and the networks topography, it could very well provide new knowledge as to how the topography would affect whether a desease will reach an endemic or pandemic state on the network.

Another area of interest would be to check whether applications of entropy in other fields could be modeled in a network and to see if the entropy behaves in the same manner. An example of this is the entropy of a chemical reaction between gases. One could, on a network, define two different populations of particles, A and B, which would react with each other to create a new particle C, $A + B \rightarrow C$ An unconstrained network would merely work as the container for these reactions, and if the right definition of the different entropies are chosen, it should behave accordingly to models

As diffusion processes has already been used to find topographical properties of networks, the entropy could provide further information to this, complementing what is already known. By running entropy simulations

on systems that have the same degree-distributions, but different clustering properties, one should expect to find some sort of relation between the time taken for the entropy to reach an equilibrium and the degree of clustering. Higher clustering would impede efficient spread of information, and should therefore give rise to longer times.

Lastly, the meaning of the dynamical entropy for a system, and what it can be used to study, is still not decided. The high importance of entropies in other systems could, however, give hope to the notion that the variable can be used to give new information to the field of networks, or in the very least, a new approach to the problems.

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