

An introduction to complex system science *

Lecture notes for the use of master and PhD students in Computer Science and Engineering

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These lecture notes are prepared as teaching material for an introductory course on Complex systems science for the use of master and PhD students in computer science and engineering. As such, they should be considered a work in progress and always under constant revision.

The field of complex systems is wide and these notes cover only a portion of it, which the author believes to be relevant for engineering and computer science curricula. Most of this teaching material is taken from the documents cited in the bibliography, with revisions and amendments. However, the author of these notes is the sole responsible for errors and inaccuracies.

*I am grateful to Prof. Silvana Bettelli Biolchini, who disclosed to me the beauty of science and introduced me to fractals, chaos and dynamical systems when I was a student at the high school. I would like to dedicate her these notes, hoping that she will enjoy reading them, remembering those pioneer times in which we had to wait a whole day to get the first fractal image on a computer monitor.

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Introduction

Complex system science (CSS) is the *corpus* of theories and methods that can help dealing with *complex systems* (CSs). Examples of complex systems are the brain, the society, the ecosystem, the cell, the ant colonies, the stock market. There is no formal definition of a complex system—and it is unlikely that a formal definition indeed exists—but we can provide a tentative, informal definition by saying that CSs are characterised by some of the following properties:

- Composed of many elements
- Nonlinear interactions
- Non-trivial network topology (i.e. not a simple structure of relations such as a tree or a star)
- Positive and negative feedbacks
- Adaptive and evolvable
- Robust
- Levels of organisation (multiscaling)

CSS has the objective of studying and modelling, and controlling CSs. It is interdisciplinary and it involves many disciplines, such as mathematics, physics, computer science, biology, economy, philosophy, neurology and more.

A peculiarity of complex systems is that local rules often propagate information in such a way that the whole system is subject to a dynamics that is not possible to understand solely on the basis of the system's constituents. Indeed, it is often said that some global behaviour *emerge* in a complex system from the interaction of its parts, governed by local rules. Despite its relevance for CSs, the concept of *emergence* remains somehow elusive. I quote below three definitions that provide a sufficiently clear framework for this phenomenon.

- “The term emergence describes the onset of novel properties that arise when a higher level of complexity is formed from components of lower complexity, where these properties are not present.” (from P.L. Luisi, *The emergence of life*, Cambridge University Press, 2006)
- “Emergence refers to the arising of novel and coherent structures, patterns, and properties during the process of self-organization in complex systems. Emergent phenomena are conceptualized as occurring on the macro level, in contrast to the micro-level components and processes out of which they arise.” (from J. Goldstein, *Emergence as a Construct*, *Emergence* 1 (1):49–72)

- “Emergence refers to all the properties that we assign to a system that are really properties of the relationship between a system and its environment.” (from Y. Bar-Yam, *Concepts in Complex Systems*, 2000. Available on the New England Complex Systems Institute website, <http://necsi.edu/guide/concepts/emergence.html>)

Strictly connected to emergence is *self-organisation*, which refers to phenomena in which some regular pattern emerges in a system, without a direct external control. Self-organization can be often observed in natural systems such as ant colonies.

Besides emergence and self-organisation, another concept that pervades CSs is *universality*, which refers to the fact that there exist behaviours appearing in many disparate systems: despite their differences at the microscopic level, some systems show the same behaviour at the macroscopic level. One of the goals of CSS is to identify the classes of local rules that generate such universal behaviours.¹

¹An very nice book illustrating “how complexity pervades biology”, and not only, is [25].

1 Systems and models

In the course of this path along some pillars of CSS, we will encounter terms that have to be defined. Often, the definition will be provided in an informal way. This is the case of the word *system*, which is usually referred to objects, things or entities (both concrete and abstract) for which it is possible to identify some kind of boundaries so that the system can be distinguished from its outside. (Of course, this is a generic definition) Therefore, once we have identified a system, it is possible to say what belongs to the system and what does not, i.e., what is outside of the system's boundaries (its environment). The identification of a system depends upon the specific level of abstraction chosen and the viewpoint of the observer. Usually, we can also say that a system is composed of other entities, whose relationships are more strong than those with the outside of the system.

The identification of systems is the first step into the study of the world around us; indeed, ancient philosophies and biology are full of discussions on systems and their classification and taxonomies. However, another concept is needed to systems' science: the *model* of a system. A model is an abstract and schematic representation of a system. It is often a formal representation of the system. It has to be emphasised that a model represents a portion of the system, as it captures only some of its features. In addition, it requires an abstraction process, which involves simplification, aggregation and omission of details.² In general, we make a model of a system to *(i)* understand it and investigate some properties, *(ii)* control it, and *(iii)* make predictions on its future. Important classes of models are differential equations and difference equations. However, in general a model can be any system we decide to use to represent another system. For example, we may want to model a biological system (e.g., a cell) by means of a computer simulation or of a wet lab experiment.

The study of general properties of systems and models is the main subject of *systems theory*.

²“Essentially, all models are wrong, but some are useful”, in Box, G.E.P., and Draper, N.R., (1987), *Empirical Model Building and Response Surfaces*, John Wiley & Sons, New York, NY, p. 424

2 Dynamical systems

A prominent class of systems concerns those systems that evolve in time. A model of a system in this class usually contains the rules that govern the time evolution of the *state* of the system. The system's state at a given time is the set of values of the magnitudes that are relevant for the system and that are somehow measurable.

It is commonly acknowledged to say that a system is *dynamical* if it can be described by models written in terms of differential or difference equations. Of course, dynamical systems can be modelled by means of other kinds of models. An excellent book on dynamical systems is [26].

Some important concepts for dynamical systems are the following:

- **Trajectory:** Sequence of states encountered during system's evolution along time. The trajectory can end at a *fixed point* or at a *cycle*, or it can be more complex (see next sections).
- **Phase space:** Space of the variables needed to characterise the system.
- **State space:** Space of the states of the system. It coincides with the phase space when the set of variables needed to characterise the system coincides with the system's state.

Typical models for dynamical systems are *ordinary differential equations* and *difference equations* (a.k.a. *iterative maps*).

2.1 Ordinary differential equations

We assume that the reader is already familiar with differential equations and in this section we summarise the main points with respect to complex dynamical systems.

Ordinary differential equations (ODE) provide a description of the evolution in time of the system's state. For example, let us consider a naive model of population growth. Let $N(t)$ be the population at time t of the species under study. The equation ruling its evolution may be:

$$\dot{N} = rN \tag{1}$$

where $r > 0$ is the growth rate. We can solve the equation analytically and obtain

$$N(t) = N_0 e^{rt} \tag{2}$$

where N_0 is the population at time $t = 0$. This equation tells that the population will grow exponentially. This is clearly not realistic, so a damping factor should be added to have a more realistic model. Indeed, when the population reaches a given level, some disadvantages usually arise due to resource competition (e.g., food and space). A correction accounting for a linear dependence between \dot{N}/N and N , leading to the **logistic**

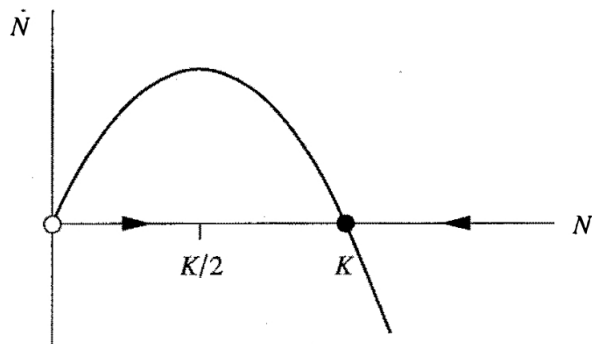


Figure 1: Picture taken from [26], p.23

equation:³

$$\dot{N} = rN \left(1 - \frac{N}{K} \right) \quad (3)$$

where K is the *carrying capacity*.

The equation can be studied analytically and the stability of its fixed points can be determined as illustrated in Box 1. Here, following [26], we study it graphically to have an idea of the qualitative behaviour of the system. We can plot \dot{N} vs. N and study the equation as if it was a vector field. From Fig.1 we can observe that the equation has two fixed points, one at $N = 0$ and the other at $N = K$. These two fixed points are the only steady states of the system. The fixed point at 0 is unstable, while the one at K is stable. The qualitative behaviour of $N(t)$ can also be derived from Fig.1 (see [26]). The study of the qualitative behaviour of Equation 3 tells us that, according to this model, a population with $N(0) > 0$ will grow fast at the beginning, then it will slow down its growing rate, until reaching a fixed point $N = K$ from which it will not move, even in front of perturbations. Should we use this model to study a real system, we would also undertake a process of *parameter tuning*, in which the parameter K and r would be set to a value such that the behaviour fit some real data. Note that, since we have required to be $r > 0$, the behaviour of $N(t)$ is qualitatively the same for every feasible value for r .

ODE are widely applied and they can be way more complicated than the logistic equation. Several branches of CSS make extensive use of differential equations, which are indeed a prominent class of models for complex systems. Another prominent class of models is that of *difference equations*, which we introduce in the next section.

³The logistic equation is able to capture some simple growth phenomena, but it has several limitations and several variants have been proposed in the literature.

Box 1: Stability of fixed points in differential equations

An analytic way to determine the stability of a fixed point x^* for a dynamical system defined by $\dot{x} = f(x)$ is the so-called *linear stability analysis*. The idea is to study the behaviour of a perturbation to x^* to see whether it decreases or increases (or keep the same value) in time. Let us consider a perturbation of the fixed point: $\eta(t) = x(t) - x^*$. The behaviour in time of $\eta(t)$ is given by $\dot{\eta}(t) = \frac{d}{dt}(x - x^*) = \dot{x}$. Thus $\dot{\eta} = f(x) = f(x^* + \eta)$. Using a Taylor series expansion we have: $\dot{\eta} = f(x^*) + \eta f'(x^*) + \mathcal{O}(\eta^2)$. By observing that $f(x^*) = 0$ and supposing that $f'(x^*) \neq 0$, the quadratic term is negligible, so we have $\dot{\eta} \approx \eta f'(x^*)$, which says that the perturbation size depends exponentially on t . Hence, the sign of $f'(x^*)$ tells us whether the perturbation is going to increase ($f'(x^*) > 0$) or decrease ($f'(x^*) < 0$).

2.2 Difference equations

Difference equations (DE) are used to model dynamical systems that update their state at discrete time steps. This class of models is widely used in the context of CS and it is particularly suitable to be studied in computer simulations. DE are of the form:

$$x(t+1) = f[x(t), P, t] \quad (4)$$

where x , f and P can be vectors and represent the state of the system, the transition functions and the parameters of the model, respectively. When a system does not depend upon t it is named *autonomous*.⁴ For a detailed description of DE in complex systems modelling (and much more!), I suggest to read the beautiful book by Serra and Zanarini, *Complex systems and cognitive processes* [19].

Let us consider the case in which we need to model a system by means of a DE. Imagine we want to design a model for the evolution in time of the number of flies in a region.⁵ The number of flies is measured once a year for a number of years, so the data we have are inherently discrete in time. The main observation is that the number of flies in year $t+1$ depends on the number of eggs laid, which in turn depends upon the number of flies in year t . As a first attempt, let us try to model the dynamics of this system with a linear DE and suppose that for each fly in generation t there will be R flies in generation $t+1$. In formulas:

$$N(t+1) = RN_t \quad (5)$$

The similarity between Eq. 5 and Eq.1 is apparent; indeed, they both model an exponential growth of the population. But there is more: Eq. 5 is the discrete-time version of Eq. 1. The qualitative behaviour of Eq. 5 can be easily studied by simulation. Once we have assigned a value to R and to $N(0)$, we iterate the map for a number of steps and we

⁴Note that this term is used also in other fields with a different meaning.

⁵This example is taken from [12].

can trace the trajectory of the system in the state space. Obviously, this is not a proof, but it helps having an idea of the behaviour of the system. There are two ways to iterate a DE: the first one is called *Cobweb method*,⁶ which is a graphical method; the second is an iterative numerical procedure, which can be conveniently implemented in a computer program.

Let us assume we want to iterate numerically the equation. The key factor in this analysis is the value of R , which induces different kinds of behaviours.

Case 1: Decay: When $0 < R < 1$ it is easy to see that the population will decay in time.

Case 2: Growth: When $R > 1$ the population increase exponentially (exponential growth).

Case 3: Steady-state behaviour: When $R = 1$ the population stays at the same level.

This simple analysis of the behaviour of the system depending on the values of the model parameters has the goal of emphasising two important points:

1. once we have designed a model it is mandatory to study its behaviour as a function of its parameters;
2. when we calibrate the parameters so as to fit real data we must pay attention to the regions in which the system will work—which may also vary in time!

As in the previous subsection, we observe that Eq. 5 is a quite rough model of the real system. Therefore, we introduce a variant that makes the offspring per fly decrease as $N(t)$ gets larger. The new equation is the so-called **logistic map**:

$$N(t + 1) = RN(t) - bN(t)^2 \tag{6}$$

where $b > 0$ rules the way in which the growth rate decreases with $N(t)$. We can transform Eq. 6 by a change of variables: be $x(t) = \frac{bN(t)}{R}$.⁷ For readability, we also change the notation by writing t as a subscript. We then obtain:

$$x_{t+1} = Rx_t(1 - x_t) \tag{7}$$

Here we assume that x_t is the fraction of individuals in the population w.r.t. the maximal population size, so it holds $x_t \in [0, 1]$.

This equation is a discrete version of Eq. 3 and we may expect that the system undergoes the same kinds of behaviour. As we will see, this is definitely not the case. To study the equation, we can draw x_{t+1} vs. x_t (see Fig.2). As we can observe, the relation is quadratic, with the maximum equal to $R/4$ at $x_t = 0.5$. We restrict the values of R to the range $[0, 4]$ so as to map x_t into itself.

⁶See [26, 12].

⁷We scale the number of flies by b/R .

Box 2: Stability of fixed points in difference equations

Given the iterative map $x_{n+1} = f(x_n)$ with a fixed point x^* , we ask if the fixed point is stable and we apply the same idea as before. The perturbation is now $\eta_n = x_n - x^*$; we have: $x^* + \eta_{n+1} = f(x^* + \eta) = f(x^*) + f'(x^*)\eta_n + \mathcal{O}(\eta_n^2)$. Since $x^* = f(x^*)$ by definition, the perturbation changes in time according to the following difference equation: $\eta_{n+1} = f'(x^*)\eta_n + \mathcal{O}(\eta_n^2)$. Thus, if $f'(x^*) \neq 0$, we have: $\eta_{n+1} \approx f'(x^*)\eta_n$. Therefore, the perturbation increases exponentially in time if $|f'(x^*)| > 1$ and decreases if $|f'(x^*)| < 1$.

By imposing $x_t = Rx_t(1 - x_t)$ we find the fixed points of the map, which are $x_1^* = 0$ and $x_2^* = (R - 1)/R$ (whenever $R \geq 1$). The stability of these fixed points can be studied as illustrated in Box 2. As expected, when $R < 1$ the only fixed point is x_1^* , which is stable. For $R > 1$ both fixed points exist, of which the first is unstable and the second is stable. However, the situation is more complicated as it seems and it can be summarised as follows.

Depending on the values of R we may observe different behaviours:

- For small values of R , i.e. $R < 1$, the population always goes extinct (Fig.3).
- For $1 < R < 3$ the population grows and eventually reaches a fixed point (Fig.4).
- For $R \geq 3$ the population oscillates (the attractor is a cycle). The period of this attractor depends on the value of R , starting from 2 and doubling while R increases (Fig.5 and Fig.6).

Let us now consider this last case of oscillating behaviour. Period doubling occurs faster and faster:

R	Period
$R_1 = 3$	2
$R_2 = 3.449\dots$	4
$R_3 = 3.54409\dots$	8
$R_4 = 3.5644\dots$	16
$R_5 = 3.568759\dots$	32
...	..
$R_\infty = 3.569946\dots$	∞

The value R_n eventually converges to the value $R_\infty \approx 3.569946$. The distance between two consecutive period doublings reduces as R increases:

$$\delta = \lim_{n \rightarrow \infty} \frac{R_n - R_{n-1}}{R_{n+1} - R_n} \approx 4.669 \quad (8)$$

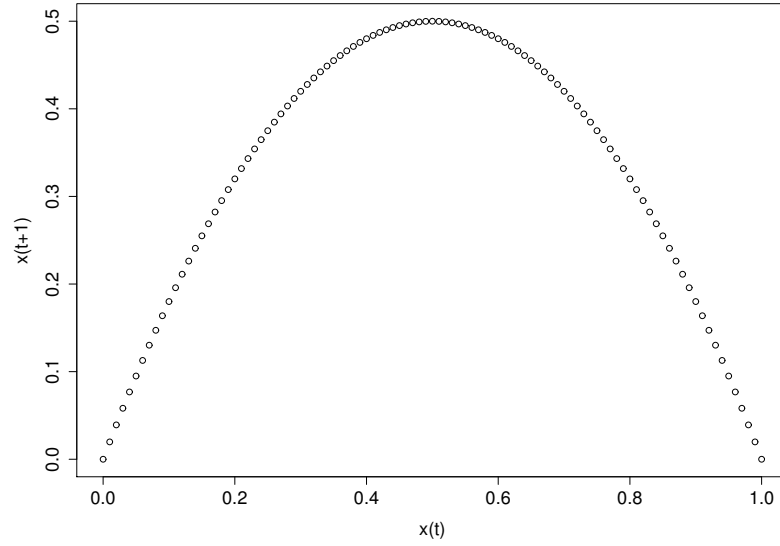


Figure 2: Graphical representation of a numerical simulation of the function x_{t+1} vs. x_t , with $R = 2$.

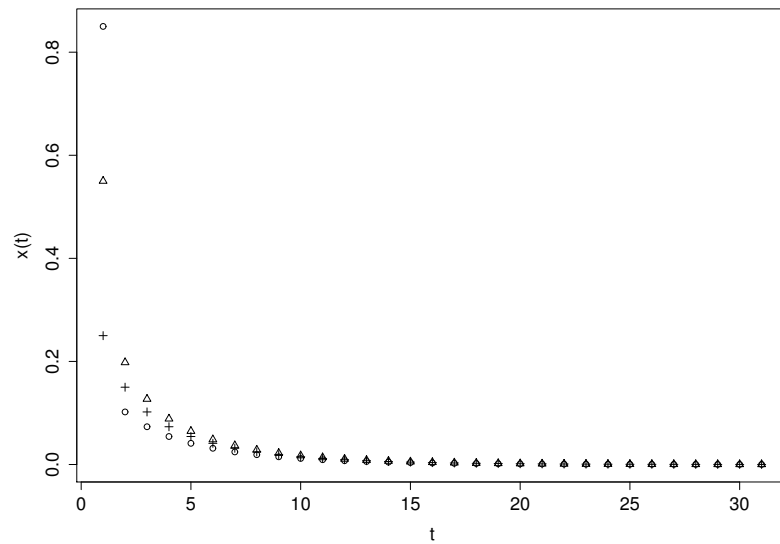


Figure 3: Graphical representation of a numerical simulation of Eq. 7 with $R = 0.8$ and $x_0 \in \{0.25, 0.55, 0.85\}$.

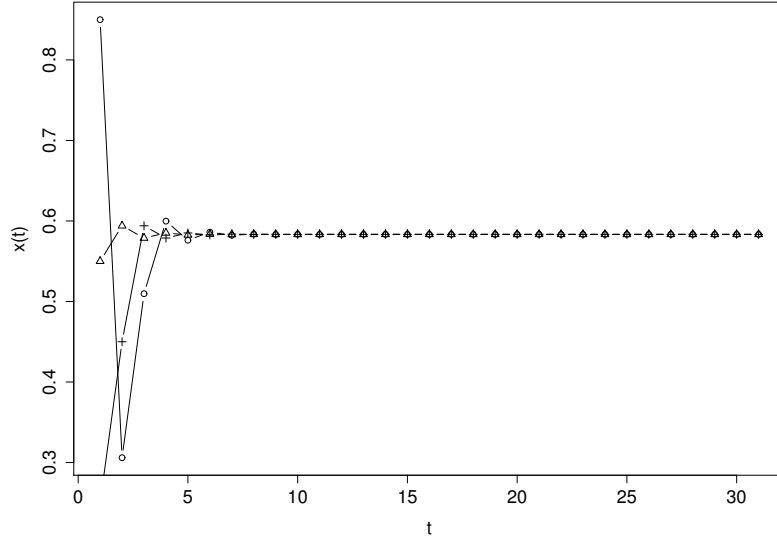


Figure 4: Graphical representation of a numerical simulation of Eq. 7 with $R = 2.2$ and $x_0 \in \{0.25, 0.55, 0.85\}$.

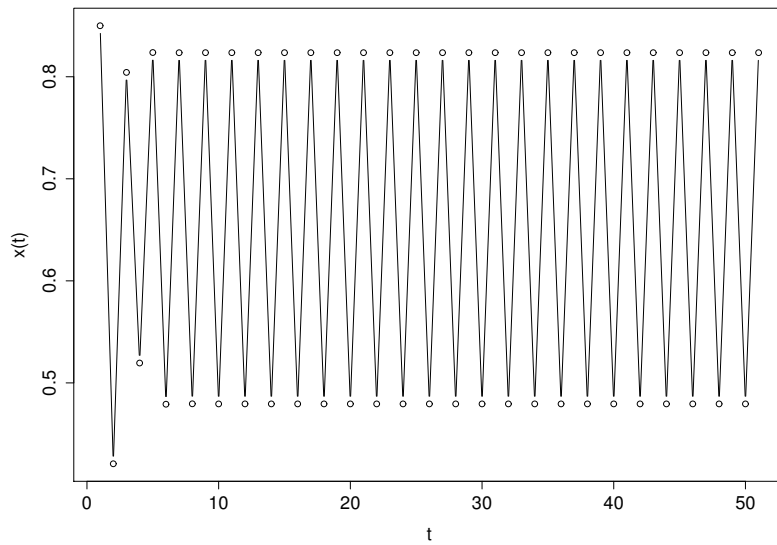


Figure 5: Graphical representation of a numerical simulation of Eq. 7 with $R = 3.3$ and $x_0 = 0.85$. The period of the cyclic attractor is 2.

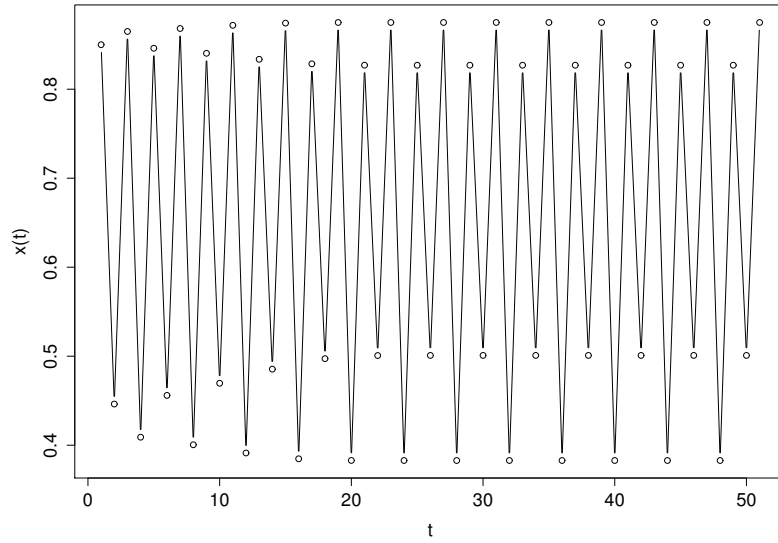


Figure 6: Graphical representation of a numerical simulation of Eq. 7 with $R = 3.5$ and $x_0 = 0.85$. The period of the cyclic attractor is 4.

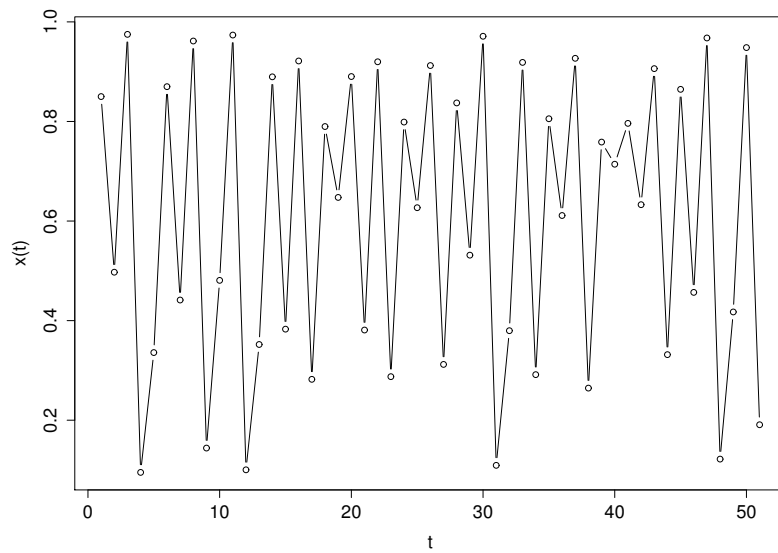


Figure 7: Graphical representation of a numerical simulation of Eq. 7 with $R = 3.9$ and $x_0 = 0.85$.

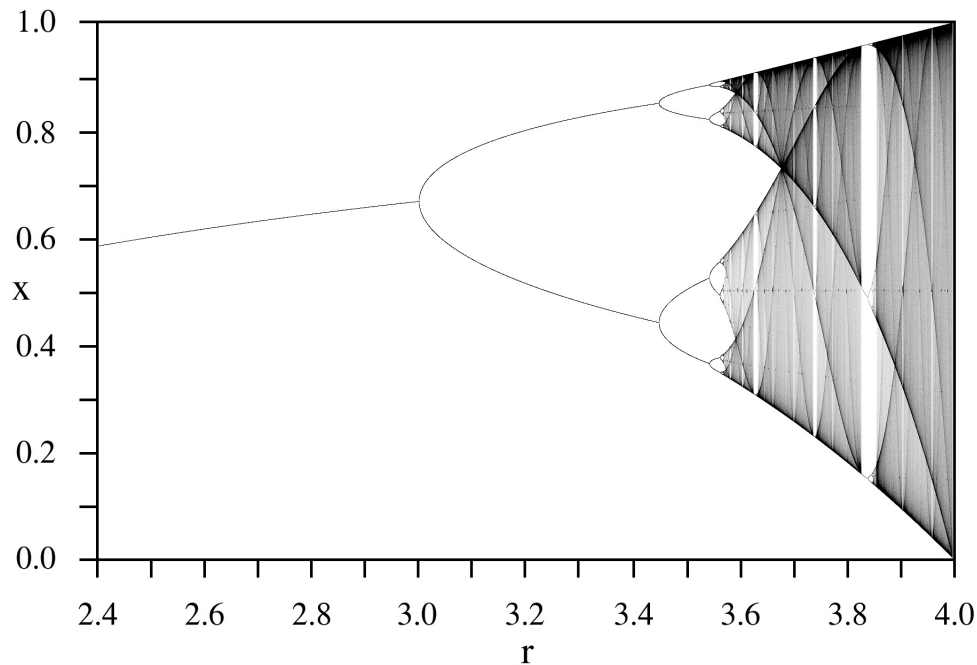


Figure 8: Bifurcation diagram for Eq. 7.

The limit is called the *Feigenbaum's number*.

We may ask now what does happen for $R > R_\infty$. In fact, something literally *strange* happens: the attractor is no longer a cycle and it seems that the trajectory randomly moves across the state space (see an example in Fig.7). A random behaviour is excluded, since the model is deterministic. So what happens? We observe a **chaotic** behaviour, which will be the subject of the next section.

Before moving to chaos, let us remark that the lesson learned from this example is that the behaviour of a system (more precisely, of the model of a system) may be dramatically different depending on the values of its parameters. A pictorial view of the different behaviours is provided by the bifurcation diagram, shown in Fig.8.

2.3 Chaos

The attractor of the system described by Eq. 7 for $R_\infty < R < 4$ is neither a fixed point, nor a cycle, but it is an attractor of different nature which is called *strange attractor*. A strange attractor seems to be random, but in fact it is not. The trajectory of the system is confined in a specific area of the phase space, but it moves in a way that is almost unpredictable. The discovery of strange attractors is attributed to Lorenz, who was working on equations for weather forecast in 1963. In Fig.9 the Lorenz's attractor is shown.

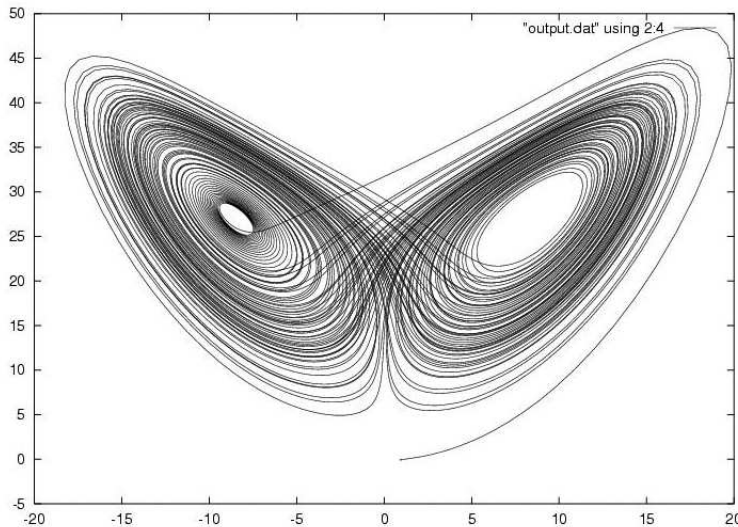


Figure 9: Lorenz's attractor.

The signature of chaos is the *sensitive dependence on initial conditions*: two nearby initial states produce trajectories that diverge exponentially in time. This property makes long term predictions very difficult, as doubling the precision in the forecast requires an increase of an order of magnitude in the precision of the measurements of the initial conditions.

The sensitivity on initial conditions can be studied analytically (for example, by means of the *Lyapunov exponent* [19]) or it can be observed also by numerical simulations. This experiment on Eq. 7 is left to the reader as an exercise.

Chaos is not random, so there should be ways to detect it, even in the cases in which we do not have access to the original model (or we are studying a real system). If we take a sample trajectory of a chaotic behaviour we can plot x_{t+1} vs. x_t . For a random map, such as $x_{t+1} = \text{Random}(0, 1)$ the plot would look like the one depicted in Fig.10. For the trajectory shown in Fig.7 we have instead the plot of Fig.11. Observe that Fig.11 represents a quite regular relation, actually like the one depicted in Fig.1. A notable case of discovery of chaotic behaviour in a real system (heart) can be found in [9].

Since its first discovery, chaos has been observed in many natural and artificial systems, from weather to electronic circuits. It is important to observe that a chaos is not a synonymous of complexity, as it will be discussed later in these notes. To know more on chaos, I suggest the book by Gleick [10].

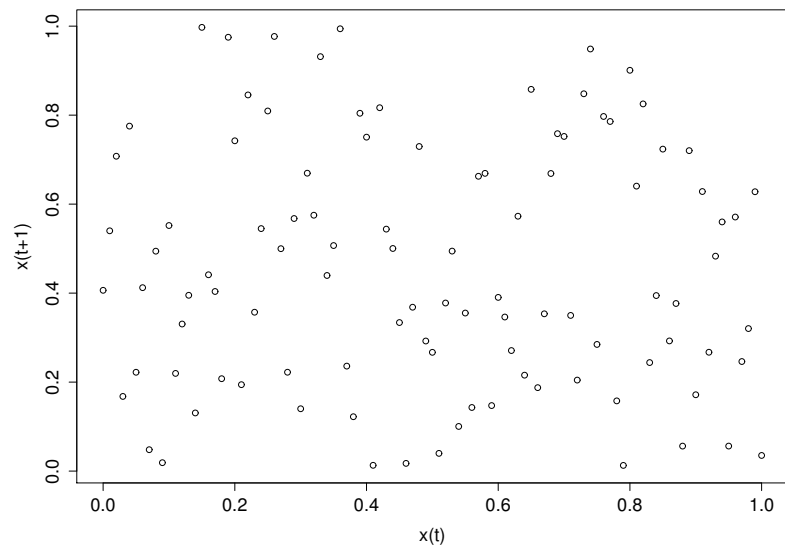


Figure 10: A random map.

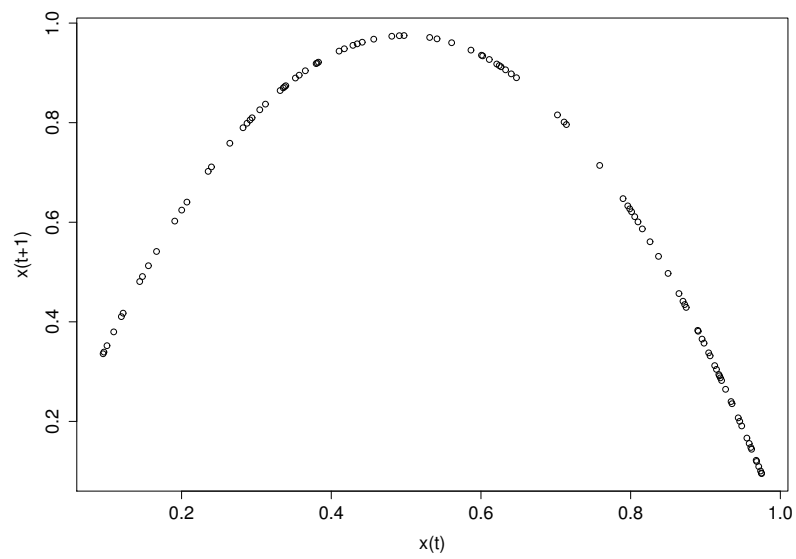


Figure 11: A chaotic map obtained from the trajectory in Fig.7.



Figure 12: The Cantor set (6 iterations of the generating procedure).

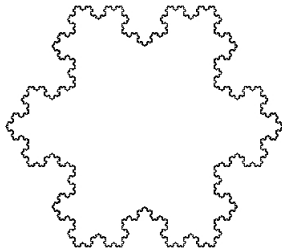


Figure 13: Koch snowflake.

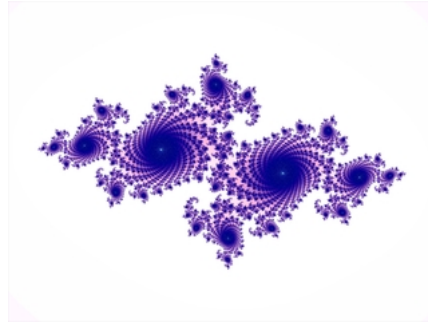


Figure 14: The Julia set.

2.4 Fractals

Strange attractors are important, as they represent situations in which predictions in a system's dynamics are rather difficult. A notable property of strange attractors is that they can be geometrically characterised as *fractals*. Fractals are geometrical objects with the following properties:⁸

- it has structure at arbitrarily small scales;
- it is self-similar;
- it has a non-integer dimension.

Self-similarity in a fractal, means that the object is composed of smaller copies of itself. As an example of a fractal, let's take the *Cantor set*. Given a segment, the Cantor set is obtained by recursively applying the following procedure: for each segment s in the set, divide s into three equal parts and delete the central one (Fig.12). The Cantor set is completely self-similar, because it is exclusively composed of smaller copies of itself.

Other examples of fractals are the Koch curve (see Fig.13) and the Julia set (see Fig.14).

By looking at these fractals, a paradox arises concerning their dimension: it seems not sound to define their dimension as the minimum number of coordinates needed to locate every point of the set, as we informally say for Euclidean objects such as segments, curves and planes. To account for a dimension of fractal objects, a more general definition is

⁸See [16].

needed. Here we introduce the *similarity dimension* [26], which we illustrate by means of some examples in the Euclidean geometry. Let's take a segment of length L : if we shrink it by 2 obtaining a segment of length $L_1 = L/2$, then we'd need 2 segments of length L_1 to obtain the first one of length L . If we shrink it by 3, then we need 3 smaller segments, and so on. Let's take a square: if we shrink it by 2 in each direction, we need 4 smaller squares to obtain the first one; if we shrink the square by 3, then we need 9 other smaller squares, and so on. In summary, we have a scale factor r and m number of copies. The *similarity dimension* is defined as follows:

$$d = \frac{\log m}{\log r} \tag{9}$$

In the case of a segment, we have $d = \frac{\log m}{\log r} = \frac{\log 2}{\log 2} = 1$. For a square: $d = \frac{\log m}{\log r} = \frac{\log 4}{\log 2} = 2$. And for a cube? $d = 3$! Now, let's calculate the dimension of the Cantor set, which is recursively given by 2 copies of a reduction by 3: $d = \frac{\log m}{\log r} = \frac{\log 2}{\log 3} \approx 0.63$. The Koch curve depicted in Fig. 13 has dimension $d = \frac{\log 4}{\log 3} \approx 1.26$.

This notion of similarity dimension can be also extended to the cases in which we do not have m and r by construction. It is based on the idea of counting the boxes needed to cover a given object.

Besides being interesting mathematical objects, fractals—and their extensions such as *multi-fractals*—provide also very useful models for real systems. Many growth phenomena are characterised by fractal properties, as well as urban development, market dynamics. In addition, fractals are applied into fields such as medical data analysis, graphics and material science.

3 Complexity: dynamical regimes between order and chaos

In the previous sections we have seen that systems can behave either quite regularly, attaining a fixed point or a cycling attractor, or they can be chaotic. However, our experience suggests us that another kind of behaviour exists, which is somehow between order and chaos. This is the realm of *complexity*, which characterises behaviours that are neither totally regular, nor completely chaotic. In a sentence, complexity lies at the edge between order and chaos [27]. CSS tries to characterise complexity, even to measure it.

In this section we illustrate the principles of complexity by means of some prominent models.

3.1 The Ising model

The Ising model is a beautiful example of a system that can exhibit both ordered and chaotic behaviours and can illustrate some important properties of the region between order and chaos. The model is a classical example in statistical physics, but here we just consider its qualitative behaviour in a simplified version, which can anyway be subject to experimental validation through computer simulations.⁹

Let's take a lattice $L \times L$ of atoms characterised by a *spin*¹⁰, which can be either up (+1) or down (-1). Each cell tends to align its spin according to the values of its first 4 neighbours, so the ideal asymptotic states of the systems are composed either of all spins up or all spins down.

The *magnetisation* of the system is defined as:

$$M = \frac{1}{N} \sum_i s_i \quad (10)$$

where s_i is the spin of atom i .

The system tries to minimise its energy, defined as follows:

$$E = - \sum_{\langle i,j \rangle} J s_i s_j \quad (11)$$

where $J > 0$ is a parameter accounting for the coupling between atoms and $\langle i, j \rangle$ denotes the set of all neighbouring pairs—counted only once.

The dynamics of the system is influenced by the temperature T : when T is low, the spins are likely to be flipped when the flip tends to align the atom with its neighbours; conversely, when T is high, spins tend to change even if their flip increases the energy.

⁹The description of the Ising model we provide here is mostly taken from [24]. The chapter containing this subject can also be downloaded as a sample chapter at: <http://press.princeton.edu/chapters/s9483.pdf>.

¹⁰The original model aims at reproducing ferromagnetic phenomena in materials.

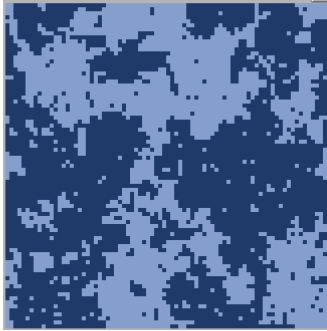


Figure 15: Ising lattice snapshot for $T \approx T_c$.

The magnetisation is called the *order parameter* of the system and the temperature is the *control parameter*.

The system can be studied analytically, but here we want to describe the main properties of the system in a qualitative way and draw some conclusions from an experimental analysis based on Monte Carlo simulation, following Algorithm 1 which represents the so-called Metropolis algorithm.

Algorithm 1 Monte Carlo simulation of a 2D Ising model. Adapted from [24].

```

while maximum number of iterations not reached do
  Choose a random atom  $s_i$ 
  Compute the energy change  $\Delta E$  associated to the flip  $s_i \leftarrow -s_i$ 
  Generate a random number  $r$  in  $[0,1]$  with uniform distribution
  if  $r < e^{-\frac{\Delta E}{kT}}$  then
     $s_i \leftarrow -s_i$ 
  end if
end while

```

The probability $e^{-\frac{\Delta E}{kT}}$ is called the *Boltzmann distribution* and k is a constant, which we assume here, for simplicity, to be equal to 1.

It is not difficult to simulate the system and observe the different dynamics of the magnetisation $M(T)$ as a function of T . For low values of T , the steady state of the system will be composed of atoms mostly frozen at the same spin and $\langle M(T) \rangle$ will be close either to 1 or -1 ; for high values of T the spins will randomly flip and it will be $\langle M(T) \rangle \approx 0$. The interesting part comes when we look at intermediate values of T , especially those close to a particular *critical* value T_c .¹¹ For values close to T_c , the magnetisation fluctuates considerably around 0 and structures emerge in the lattice (see Fig. 15). At $T = T_c$ a *phase transition* occur: the system magnetisation undergoes a change in its possible steady state values, as depicted in Fig. 16.

The main properties arising in general at the critical point are the following:

¹¹It can be proven that $T_c = 2.27$.

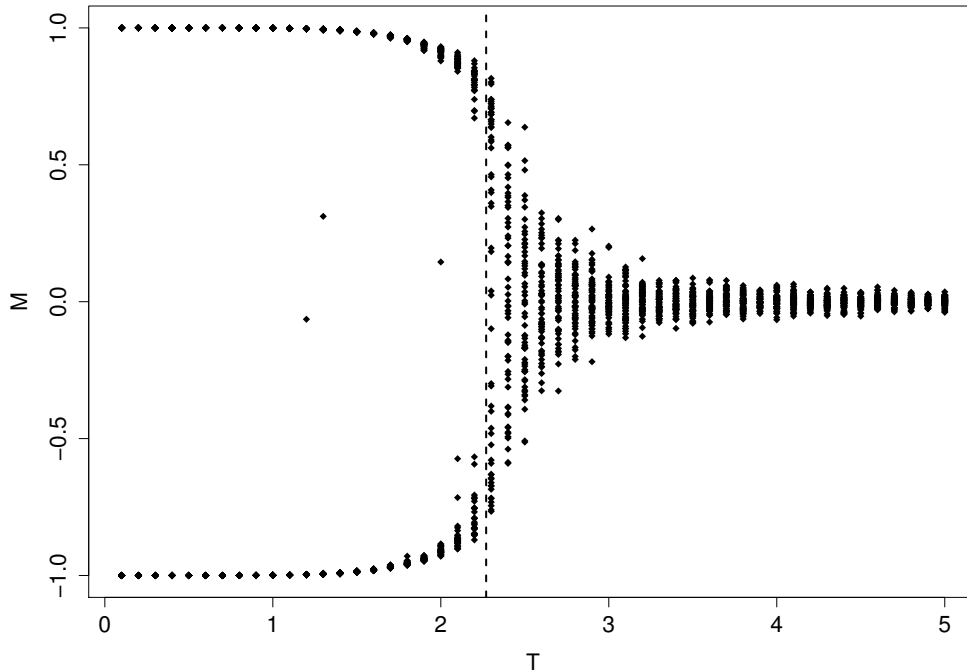


Figure 16: Bifurcation diagram for the 2D Ising model obtained by a Monte Carlo simulation of a 30×30 lattice. Dashed vertical line at $T = T_c = 2.27$

- Large fluctuations
- Long-range correlations
- Percolation
- Scale-free ($1/f$)

These properties will be discussed in more detail in the following sections. Here we just remark that in the proximity of the critical point (of the control parameter), the order parameter has large fluctuations, as depicted in Fig. 17. This phenomenon suggests to use special care when we deal with system in a dynamical regime between order and chaos/randomness.

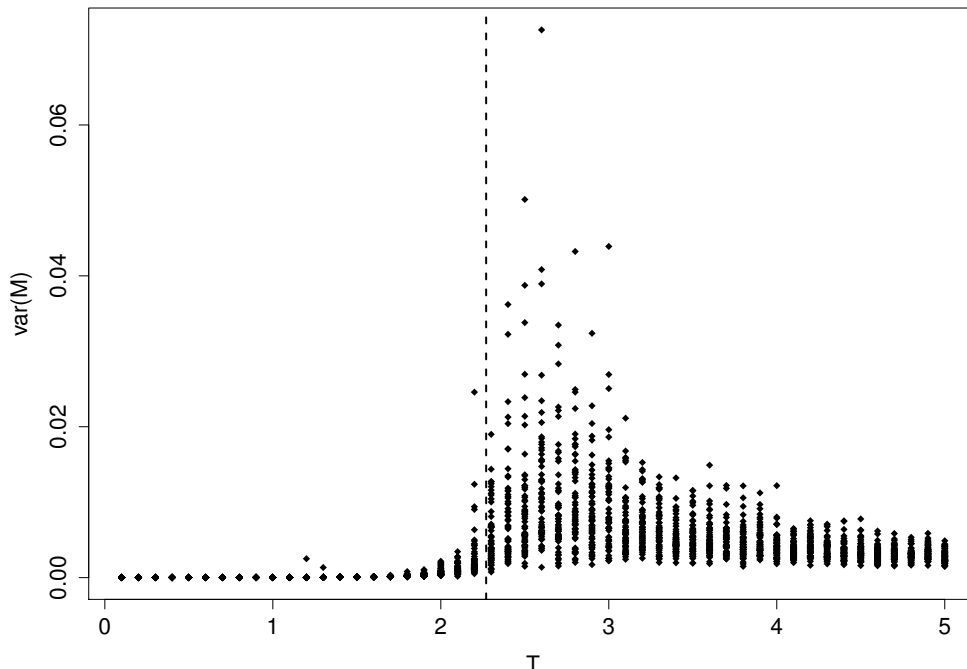


Figure 17: Variance of the average magnetisation values of Fig. 16. The shift w.r.t. T_c is due to the approximation introduced by the numerical estimations (length of transient and of the time range for computing the averages).

3.2 Phase transitions, symmetry breaking and behaviour changes

In the previous subsection, we have informally introduced the fundamentals of phase transitions by means of the Ising model. The phase transition observed is of the *second order*, i.e., the order parameter changes continuously as the control parameter is varied. Indeed, what changes is not the dynamics of the single instance of the spin system, but rather the possible future steady states of an ensemble of spin system instances.

The analogous of this ensemble phenomenon for a single dynamical system is called a *bifurcation*, which denotes the situations in which a system can exhibit qualitative changes with respect to the variation of some control parameters. Examples are the propagation of fire, information or viruses depending on a propagation threshold, and the change in the structure of a system, such as the shift from vegetated to desert habitats.

Mathematically, a bifurcation corresponds to the appearance—and disappearance—of new steady states, sometimes alternative. It is important to emphasise that in these latter cases, the final attractor of the system is *path dependent*, i.e., it is sensitive to initial conditions and little fluctuations in the transient. A pictorial view of this phenomenon is provided in Figure 18, in which a ball can follow different paths depending on small

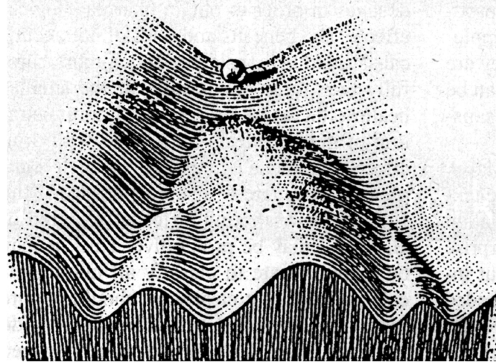


Figure 18: The epigenetic landscape. Picture taken from Slack, J.M.W., Conrad Hal Waddington: the last Renaissance biologist?, Nature, vol. 3, November 2002.

fluctuations on its initial condition or along its trajectory, up to a point from which on it will be trapped in one of the possible future dynamics.

Bifurcations can be illustrated by simple mathematical examples, such as the following differential equation:

$$\frac{dx}{dt} = \mu x - x^3 = f_\mu(x) \quad (12)$$

The fixed points of the system are $0, +\sqrt{\mu}, -\sqrt{\mu}$; of course depending on the sign of μ we can have either one or three fixed points. The stability of a fixed point x^* can be determined by checking the sign of $\left. \frac{df_\mu}{dx} \right|_{x^*} = \mu - x^{*2}$. Hence, for $\mu < 0$, the only fixed point is $x^* = 0$, which is stable (see Figure 19). For $\mu > 0$, the point 0 becomes unstable, whilst the new fixed points $\pm\mu$ are stable (see Figure 20). The properties of the steady states of the system can be represented by a bifurcation diagram, as depicted in Figure 21.

The phenomenon of symmetry breaking can be understood also by means of a *potential function* $\Phi_\mu(x)$, defined by the following equation:

$$f_\mu(x) = -\frac{\Phi_\mu(x)}{dx} \quad (13)$$

If we suppose that the hypothesis of integrability of $f_\mu(x)$ is valid—which is indeed our case—then we have:

$$\Phi_\mu(x) = -\frac{\mu}{2}x^2 + \frac{1}{4}x^4 \quad (14)$$

The function $\Phi_\mu(x)$ is depicted for several values of μ in Figure 22 ($\mu = 1$), Figure 23 ($\mu = 0.1$) and Figure 22 ($\mu = -1$). The extrema of $\Phi_\mu(x)$ corresponds to the fixed points of $f_\mu(x)$ and the second derivative of $\Phi_\mu(x)$ characterises the stability of fixed points. (Note that the metaphor of a ball rolling down a smooth surface matches quite well the mathematical intuition)

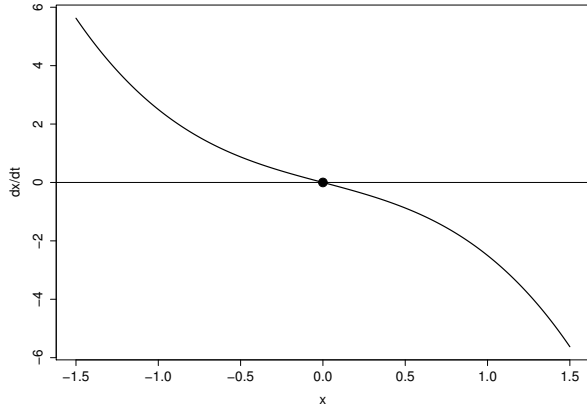


Figure 19: $f_{\mu}(x)$ for $\mu = -1$

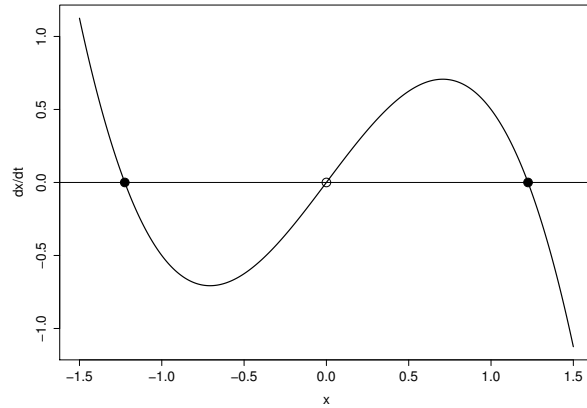


Figure 20: $f_{\mu}(x)$ for $\mu = 1.5$

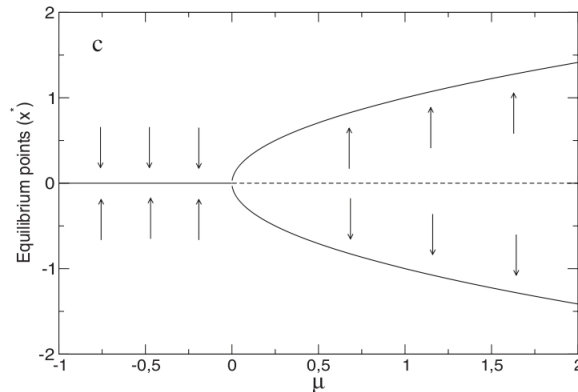


Figure 21: Bifurcation diagram of the system described by Eq. 12. Picture taken from [24].

As we can observe, the system can undergo two kinds of steady-state behaviours, depending on the sign of μ . Moreover, note that for $\mu > 0$ the system can reach either of two fixed points, so in a sense it has to decide between two alternatives.

Symmetry breaking is also typical of complex systems exhibiting self-organisation—e.g., ants in foraging behaviour choosing between two paths of equal length. Therefore, we can understand the meaning of the critical point (in this case, $\mu = 0$): both in the case of a phase transition in systems composed of many elements and in mathematical bifurcations, the critical point separates two different kinds of system's behaviour. It is also interesting to observe what happens for values of μ close to the critical value: the potential is flat in the vicinity of 0, so a small perturbation might move the system far away from the initial point before it can return to the stable fixed point. This is a property typical of systems close to a critical phase: a perturbation takes very long to get dampened. This is also

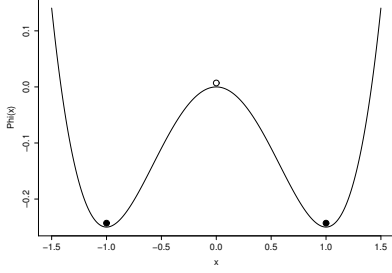


Figure 22: $\Phi_\mu(x)$ for $\mu = 1$.

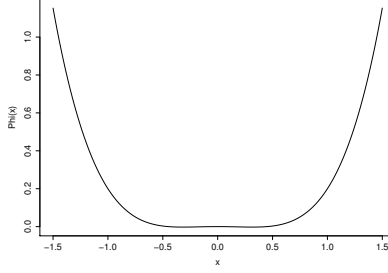


Figure 23: $\Phi_\mu(x)$ for $\mu = 0.1$.

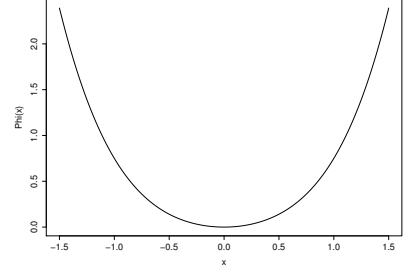


Figure 24: $\Phi_\mu(x)$ for $\mu = -1$.

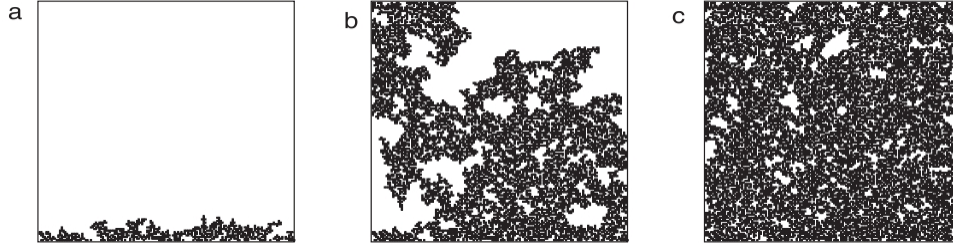


Figure 25: Fire behaviour in forests at different density p . (a) $p < p_c$; (b) $p = p_c$; (c) $p > p_c$. Picture taken from [24].

a consequence of the fact that in critical systems, information exchange takes part also between “distant” parts of the systems.

3.3 Examples

In general, we are interested in those situations in which the system can undergo qualitative changes as a function of some control parameters. In this section, we briefly review some notable examples.

3.3.1 Forest-fire model

A relevant property of many critical systems is *percolation*, i.e., the phenomenon in which information flows across the whole system. In situations in which percolation occurs, the system assumes a particular structure in which its elements form connected islands of activity.

A case in point is the forest-fire model: the simplest model is provided by a lattice in which cells can be either occupied by a tree or empty. Cells are initially assigned by means of a Bernoulli distribution of parameter p . If all the trees of a given edge of the lattice are

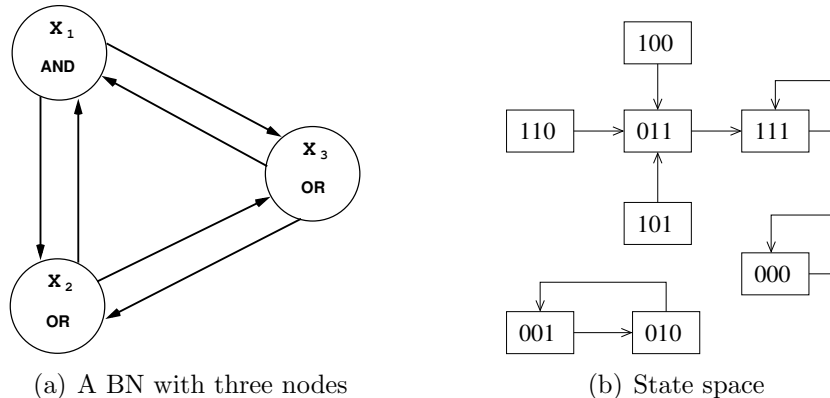


Figure 26: An example of a BN with three nodes (a) and its corresponding state space under synchronous and deterministic update (b). The network has three attractors: two fixed points, $(0, 0, 0)$ and $(1, 1, 1)$, and a cycle of period 2, $\{(0, 0, 1), (0, 1, 0)\}$.

burned, then fire spreads across the lattice depending on the density of the trees. Below a critical value of p ($p_c \approx 0.59$), the fire dies quickly, as trees are sparse; instead, above p_c the fire reaches the whole area very fast because trees are dense. At $p = p_c$ there is a phase transition, in which the control parameter is p and the order parameter is the fraction of burned trees (see Figure 25).

An important property of the system at $p = p_c$ is that the fire percolates across the system, i.e., it spans the whole system but leaves some “holes” at all scales; the set of burned trees at p_c composes a fractal object.

It is interesting to remark that at the critical point there is an abrupt transition in fire spreading: for $p > p_c$ the fire, i.e., information, pervades the whole system. This property is typical of many complex phenomena.

3.3.2 Random Boolean networks

Boolean networks (BNs) have been introduced by Kauffman [13, 14] as a genetic regulatory network model. BNs have been proven to reproduce very important phenomena in genetics and they have also received considerable attention in the research communities on complex systems [2, 14]. A BN is a discrete-state and discrete-time dynamical system whose structure is defined by a directed graph of N nodes, each associated to a Boolean variable x_i , $i = 1, \dots, N$, and a Boolean function $f_i(x_{i_1}, \dots, x_{i_{K_i}})$, where K_i is the number of inputs of node i . The arguments of the Boolean function f_i are the values of the nodes whose outgoing arcs are connected to node i (see Figure 26a). The state of the system at time t , $t \in \mathbb{N}$, is defined by the array of the N Boolean variable values at time t : $s(t) \equiv (x_1(t), \dots, x_N(t))$. The most studied BN models are characterised by having a *synchronous* dynamics—i.e., nodes update their states at the same instant—and *deterministic* functions (see Figure 26b). However, many variants exist, including asynchronous

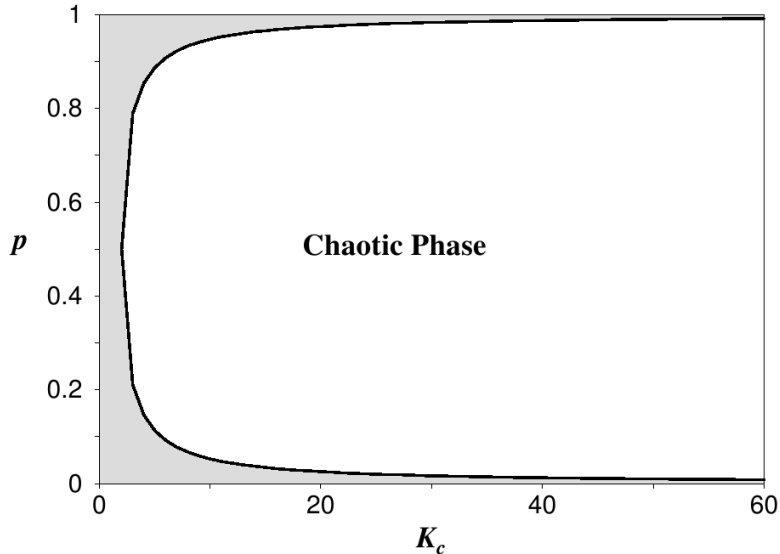


Figure 27: Critical line for RBNs, as a function of p and K .

and probabilistic update rules [22].

BN models' dynamics can be studied by means of usual dynamical systems methods, hence the usage of concepts such as state (or phase) space, trajectories, attractors and basins of attraction. BNs can exhibit complex dynamics and some special ensembles have been deeply investigated, such as that of Random BNs. Recent advances in this research field, along with efficient mathematical and experimental methods and tools for analysing BN dynamics, can be mainly found in works addressing issues in genetic regulatory networks or investigating properties of BN models.

A special category of BNs that has received particular attention is that of RBNs, which can capture relevant phenomena in genetic and cellular mechanisms and complex systems in general. RBNs are usually generated by choosing at random K inputs per node and by defining the Boolean functions by assigning to each entry of the truth tables a 1 with probability p and a 0 with probability $1 - p$. Parameter p is called *bias*. Depending on the values of K and p the dynamics of RBNs is called either *ordered* or *chaotic*. In the first case, the majority of nodes in the attractor is frozen and any moderate-size perturbation is rapidly dampened and the network returns to its original attractor. Conversely, in chaotic dynamics, attractor cycles are very long and the system is extremely sensitive to small perturbations: slightly different initial states lead to divergent trajectories in the state space.

RBNs temporal evolution undergo a second order phase transition between order and chaos, governed by the following relation between K and p : $K_c = [2p_c(1 - p_c)]^{-1}$, where the subscript c denotes the critical values [7] (see Figure 27). Networks along the critical line show equilibrium between robustness and adaptiveness [1]; for this reason they are supposed

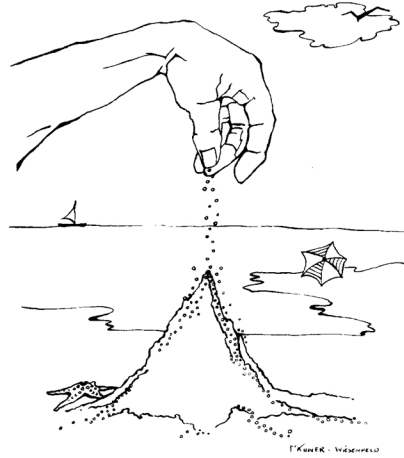


Figure 28: A pictorial view of the sand pile model. Picture taken from [3].

to be plausible models of the living systems organisation. Recent results support the view that biological genetic regulatory networks operate close to the critical region [18, 23, 5].

3.4 Self-organised criticality

Now a question arises as to why so many real systems are critical. The answer is not unique and still incomplete. However, we can say that some reasons for this phenomenon are connected with robustness and evolvability, others are to be found in the fact that criticality seems to be connected with a maximal information processing capability. A further reason is provided by the theory of *self-organised criticality* (SOC).

SOC has been proposed by Bak [4, 3]. Succinctly, the theory states that many systems naturally evolve toward a critical attractor, i.e., an attractor at a phase transition. The interesting point here is that there is no need of tuning a control parameter, but rather it is the system that evolves toward this critical point. Self-organised critical systems are not in equilibrium and possess many degrees of freedom. Examples of SOC can be found in earthquakes, solar flares, evolutionary models, economic and social behaviours, just to mention some examples.

SOC can be easily illustrated by the so-called *sand pile model*. Let us consider a device that periodically drops one sand grain at a time from the same position: grains fall down one over the other and create a pile (see Figure 28). While the pile grows, from time to time we observe avalanches, which are normally distributed and small on average. But, once a certain size of the pile is reached, avalanches are distributed according to a power law, i.e., there are avalanches of every intensity (see Figure 29). A system with this property is said to be *scale-free*. The pile can not grow over but it also can not stop the addition of grains, so it “reacts” by showing this behaviour which is a stable attractor.

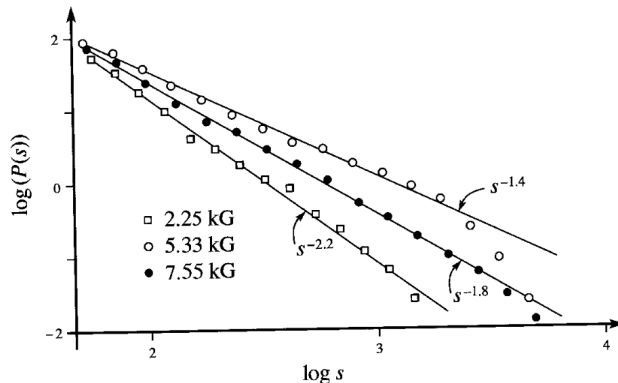


Figure 29: Distribution of earthquakes of given energy. The probability $P(s)$ of finding an earthquake of size s goes approximately as $s^{-\gamma}$. Picture taken from [3].

4 Information-theoretic measures in CSS

In the study of complex systems we frequently resort to qualitative descriptions to identify some properties of a system. One reason is that some concepts, even though widely used since decades, are still elusive. Examples are the concepts of self-organisation and emergence, not to mention complexity itself. In this section, we will succinctly present some measures that can be usefully applied to quantify some properties of dynamical systems. The root of these measures is information theory.¹² The link between complex systems and information theory is the fact that a computational process can be seen as the evolution in time of a dynamical system. Thus, some properties of the system can be conveniently studied by means of information-theoretic measures.

4.1 Information entropy

The first notion to be considered is (*information*) *entropy*, introduced by Shannon in 1948.¹³

Let us consider a simple system of which we observe the state at a given time. The observation can be modelled as a random variable X which can assume values from a finite and discrete domain \mathcal{X} . If the observation is $x \in \mathcal{X}$, which has a probability $P(x)$, then the information content of the observation is measured as $\frac{1}{\log_2 P(x)} = -\log_2 P(x)$.¹⁴ An improbable observation conveys more information than one associated to high probability.

¹²For a detailed and profound discussion on these subjects, I suggest to read the *Information theory for complex systems* lecture notes by Prof. Kristian Lindgren, <http://studycas.com/c/courses/it>, visited on April 2014. For a quick overview on the subject, see [17].

¹³The measure is also called the Shannon entropy.

¹⁴The usual unity measure in information theory is the bit, so logarithms are in base 2. Hereafter, we will omit the base in the mathematical notation.

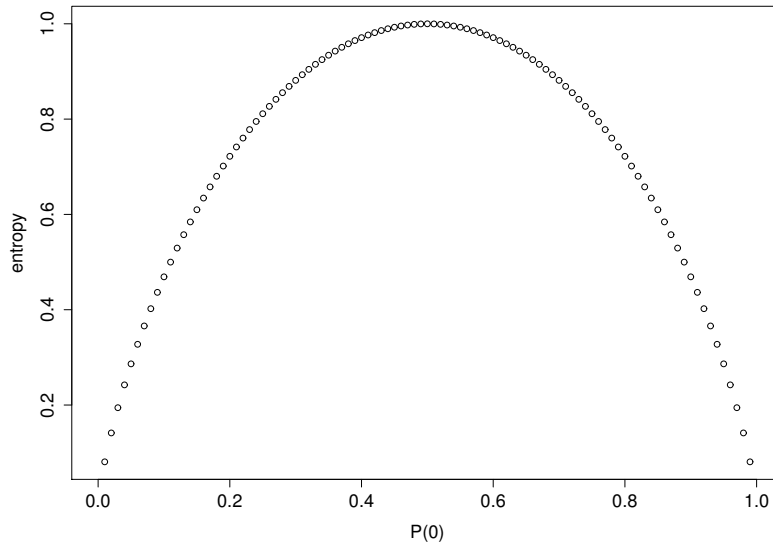


Figure 30: Entropy values for a Bernoulli distributed stochastic variable.

We can characterise the system by averaging over its possible outcomes:

$$H(X) = - \sum_{x \in \mathcal{X}} P(x) \log P(x) \quad (15)$$

In the definition of $H(X)$ we assume $0 \log 0 = 0$.

Intuitively, $H(X)$ measures the degree of randomness of the process. For example, let's consider the case of a pure random binary variable: we have $\mathcal{X} = \{0, 1\}$ and $P(0) = P(1) = 0.5$. Hence, $H(X) = -2(0.5 \log(0.5)) = 1$. In general, for n symbols appearing with equal probability, we have $H(X) = \log(n)$, which is the maximum value. Conversely, if $P(0) \approx 1$ (so $P(1) = 1 - P(0) \approx 0$), the entropy is quite small, as it is very likely that X will assume value 0 (see Figure 30). Therefore, a high entropy characterises systems that show string tendency to disorder, whilst it is low for ordered systems.

Example: entropy of the Ising model

Let's consider the Ising model, as defined in Section 3.1. An estimation of its information content can be given by computing the average atom entropy. For atom S_i , the probability of occurring with spin -1 , is estimated by computing the frequency of occurrence of spin -1 in the series of states collected. As we can observe in Figure 31, the average entropy is low for low temperature values and high for high temperatures. Note that the relation is nonlinear, with a sharp increase at the phase transition.

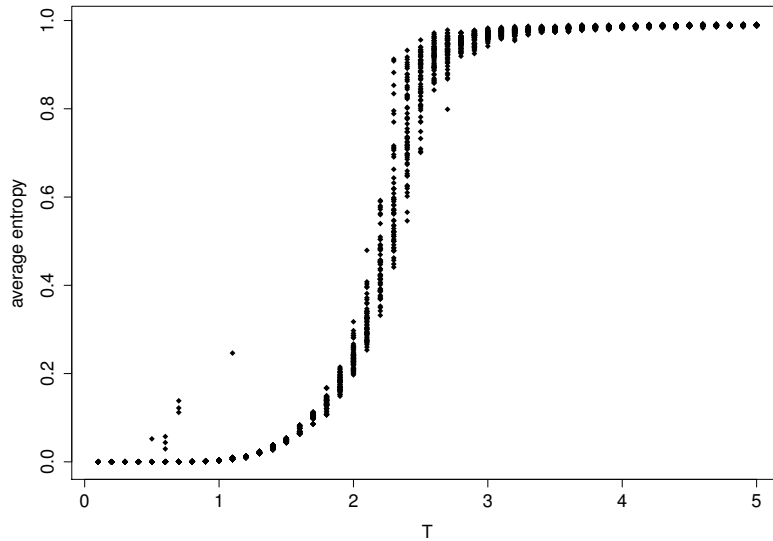


Figure 31: Average entropy for a 30×30 Ising model, as a function of T .

4.2 Related information measures

Entropy is the base for computing other important information-theoretic measures.

First of all, this definition can be extended to blocks of symbols of length n in s , so as to take into account also correlations among symbols. This leads to the definition of the *block entropy* of length n :

$$H_n = - \sum_{s_n \in \mathcal{S}} P(s_n) \log P(s_n)$$

The *entropy excess*¹⁵ is defined as the difference between block entropies of length n and $n - 1$ and estimates the information required to predict the n -th symbol conditioned to the observation of $n - 1$ preceding symbols. In formulas:

$$h_n = \Delta H_n = H_n - H_{n-1}$$

We can extend this process to the second derivative (in discrete domains) and obtain the *correlation information* from length n :

$$k_n = \Delta^2 H(n) = -H(n) + 2H(n - 1) - H(n - 2), \quad n \geq 3$$

Intuitively, the peaks of k_n identify significant block regularities, i.e. maximum gain in information for specific block lengths.

¹⁵Not to be confused with the *excess entropy* [21], which is defined for $n \rightarrow \infty$.

Also the *mutual information* $I(X, Y)$ between random variables X and Y is defined in terms of entropies and estimates the average information one gains about Y after the observation of X , and viceversa:

$$I(X, Y) = H(X) + H(Y) - H(X, Y)$$

where $H(X, Y)$ denotes the conjunct entropy of X and Y .

A generalisation of the mutual information is the so-called *integration* (a.k.a. *intrinsic information* or *multi-information*):

$$I(X_1; X_2; \dots; X_k) = \sum_{i=1}^k H(X_i) - I(X_1, X_2, \dots, X_k) \quad (16)$$

4.3 Algorithmic complexity

The notion of entropy suggests to focus on the amount of disorder of a system and it can be computed by estimating the probabilities of occurrence of the symbols produced. A related measure does not require to know this probability distribution and relies on computability principles. The algorithmic complexity of a sequence of symbols refers to the length in bits of the minimal program that generates the sequence, without input. This measure is known as *Kolmogorov complexity* (KC). For example, the sequence 01010101...01 has low KC, while a random generated sequence of bits has the highest value of KC.

The KC can not be computed exactly, but it can be estimated, for example by means of compression algorithms. Note that a high compression ratio means that the sequence contains high regularity, while low compression ratio might be the signal of randomness. Of course, these estimations should be taken *cum grano salis*, because they depend on the compression algorithm used.

4.4 Statistical complexity

We could be satisfied with the previous measures to study the system, but in fact they do not capture the intuitive notion of complexity, as a property characterising systems at the edge of order and disorder. A random sequence of symbols 0 and 1 should be evaluated with low complexity, rather than its maximum. To overcome this problem, several measures as been proposed [17] to account for *statistical complexity* (SC), i.e., the algorithmic complexity of a program that reproduces the statistical properties of a system. In this light, the SC of a random sequence is low.

Among various measures of SC, we mention a simple yet effective one, which is called LMC complexity, by the name of its inventors [15]. The idea is rather simple: if we want the SC of a system to be high in intermediate regions between order and disorder, we can define a measure as the product of a measure that increases with disorder and another

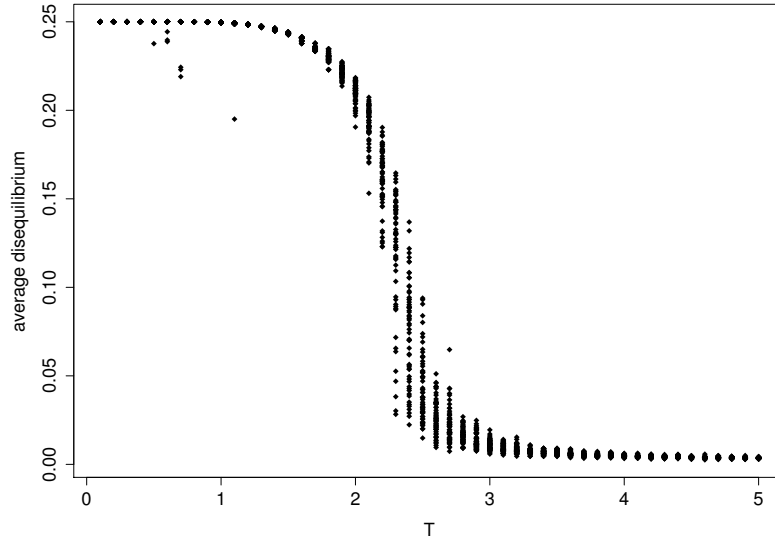


Figure 32: Average disequilibrium for a 30×30 Ising model, as a function of T .

which decreases with it. We know that entropy measures disorder, this is the former factor. The second can be the *disequilibrium*:

$$D(X) = \sum_{x \in \mathcal{X}} \left(P(x) - \frac{1}{|\mathcal{X}|} \right)^2 \quad (17)$$

The disequilibrium estimates the extent to which a system exhibits patterns far from equidistribution. For example, if the trajectory of a system is composed of only few of the possible states (e.g., a short cyclic attractor), then it has a high disequilibrium.

The LMC complexity is defined as: $LMC(X) = H(X) \cdot D(X)$.

Example: LMC complexity of the Ising model

Let us computed the LMC complexity for the Ising model, as previously done for the entropy. Results for the disequilibrium and LMC complexity are depicted in Figure 32 and Figure 33, respectively. As we can observe, the shape of the LMC complexity shows a remarkable peak at the phase transition, exactly where criticality resides.

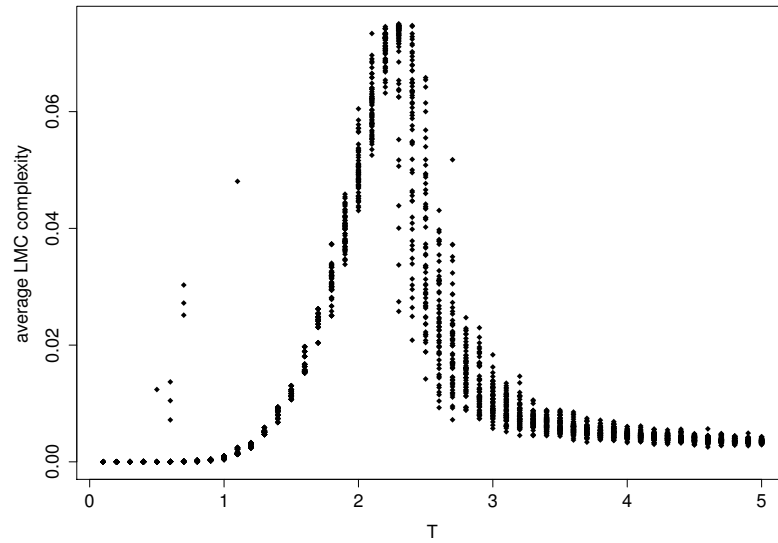


Figure 33: Average LMC complexity for a 30×30 Ising model, as a function of T .

Further notes on complexity measures

Measuring complexity is still an elusive task and it is tightly entangled with the formal characterisation of emergence and self-organisation. The discussion of this extremely relevant topic is not in the scope of these lectures, so I just suggest some references to know more on the subject [8, 11, 6, 20, 17].

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