

# Introduction to Complex Systems

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## 1.1 Physics, biology, or social science?

The science of complex systems is not an offspring of physics, biology, or the social sciences, but a unique mix of all three. Before we discuss what the science of complex systems is or is not, we focus on the sciences from which it has emerged. By recalling what physics, biology, and the social sciences are, we will develop an intuitive feel for complex systems and how this science differs from other disciplines. This chapter thus aims to show that the science of complex systems combines physics, biology, and the social sciences in a unique blend that is a new discipline in its own right. The chapter will also clarify the structure of the book.

## 1.2 Components from physics

Physics makes quantitative statements about natural phenomena. Quantitative statements can be formulated less ambiguously than qualitative descriptions, which are based on words. Statements can be expressed in the form of predictions in the sense that the trajectory of a particle or the outcome of a process can be anticipated. If an experiment can be designed to test this prediction unambiguously, we say that the statement is experimentally testable. Quantitative statements are validated or falsified using quantitative measurements and experiments.

Physics is the experimental, quantitative, and predictive science of matter and its interactions.

Pictorially, physics progresses by putting specific questions to nature in the form of experiments; surprisingly, if the questions are well posed, they result in concrete answers that are robust and repeatable for an arbitrary number of times by anyone who can do the same experiment. This method of generating knowledge about nature, by using experiments to ask questions of it, is unique in the history of humankind and is called the *scientific method*. The scientific method has been at the core of all technological progress since the time of the Enlightenment.

Physics deals with matter at various scales and levels of granularity, ranging from macroscopic matter like galaxies, stars, planets, stones, and projectiles, to the scale of molecules, atoms, hadrons, quarks, and gauge bosons. There are four fundamental forces at the core of all interactions between all forms of matter: gravity, electromagnetism and two types of nuclear force: the weak and the strong. According to quantum field theory, all interactions in the physical world are mediated by the exchange of gauge bosons. The graviton, the boson for gravity, has not yet been confirmed experimentally.

### 1.2.1 The nature of the fundamental forces

The four fundamental forces are very different in nature and strength. They are characterized by a number of properties that are crucial for understanding how and why it was possible to develop physics without computers. These properties are set out here.

Usually, the four fundamental forces are homogeneous and isotropic in space (and time). Forces that are homogeneous act in the same way everywhere in space; forces that are isotropic are the same, regardless of the direction in which they act. These two properties drastically simplify the mathematical treatment of interactions in physics. In particular, forces can be written as derivatives of potentials, two-body problems can effectively be treated as one-body problems, and the so-called mean field approach can be used for many-body systems. The mean field approach is the assumption that a particle reacts to the single field generated by the many particles around it. Often, such systems can be fully understood and solved even without computers. There are important exceptions, however; one being that the strong force acts as if interactions were limited to a ‘string’, where flux-tubes are formed between interacting quarks, similar to type II superconductivity.

The physical forces differ greatly in strength. Compared to the strong force, the electromagnetic force is about a thousand times weaker, the weak force is about  $10^{16}$  times weaker, and the gravitational force is only  $10^{-41}$  of the strength of the strong force [405]. When any physical phenomenon is being dealt with, usually only a single force has to be considered. All the others are small enough to be safely neglected. Effectively, the superposition of four forces does not matter; for any phenomenon, only one force

Matter	Interaction types	Characteristic length scale
macroscopic matter	gravity, electromagnetism	all ranges
molecules	electromagnetism	all ranges
atoms	electromagnetism, weak force	$\sim 10^{-18}$ m
hadrons and leptons	electromagnetism, weak and strong force	$10^{-18} - 10^{-15}$ m
quarks and gauge bosons	electromagnetism, weak and strong force	$10^{-18} - 10^{-15}$ m

is relevant. We will see that this is drastically different in complex systems, where a multitude of different interaction types of similar strength often have to be taken into account simultaneously.

Typically, physics does not specify which particles interact with each other, as they interact in identical ways. The interaction strength depends only on the relevant interaction type, the form of the potential, and the relative distance between particles. In complex systems, interactions are often *specific*. Not all elements, only certain pairs or groups of elements, interact with each other. Networks are used to keep track of which elements interact with others in a complex system.

### 1.2.2 What does predictive mean?

Physics is an experimental and a predictive science. Let us assume that you perform an experiment repeatedly; for example, you drop a stone and record its trajectory over time. The predictive or theoretical task is to predict this trajectory based on an understanding of the phenomenon. Since Newton's time, understanding a phenomenon in physics has often meant being able to describe it with differential equations. A phenomenon is understood dynamically if its essence can be captured in a differential equation. Typically, the following three-step process is then followed:

1. Find the differential equations to encode your understanding of a dynamical system. In the example of our stone-dropping experiment, we would perhaps apply Newton's equation,

$$m \frac{d^2 x}{dt^2} = F(x),$$

where  $t$  is time,  $x(t)$  is the trajectory,  $m$  is mass of the stone, and  $F$  is force on the stone. In our case, we would hope to identify the force with gravity, meaning that  $F = gm$ .

2. Once the equation is specified, try to solve it. The equation can be solved using elementary calculus, and we get,  $x(t) = x_0 + v_0 t + \frac{1}{2} g t^2$ . To make a testable prediction we have to fix the boundary or initial conditions; in our case we have to specify what the initial position  $x_0$  and initial velocity  $v_0$  are in our experiment. Once this is done, we have a prediction for the trajectory of the stone,  $x(t)$ .
3. Compare the result with your experiments. Does the stone really follow this predicted path  $x(t)$ ? If it does, you might claim that you have understood something on a quantitative, predictive, and experimental basis. If the stone (repeatedly) follows another trajectory, you have to try harder to find a better prediction.

Fixing initial or boundary conditions means simply taking the system out of its context, separating it from the rest of the universe. There are no factors, other than the boundary conditions, that influence the motion of the system from the outside. That

such a separation of systems from their context is indeed possible is one reason why physics has been so successful, even before computing devices became available. For many complex systems, it is impossible to separate the dynamics from the context in a clear way. This means that many outside influences that are not under experimental control will simultaneously determine their dynamics.

In principle, the same thinking used to describe physical phenomena holds for arbitrarily complicated systems. Assume that a vector  $X(t)$  represents the state of a system at a given time (e.g. all positions and momenta of its elements), we then get a set of equations of motion in the form,

$$\frac{d^2 X(t)}{dt^2} = G(X(t)),$$

where  $G$  is a high-dimensional function. Predictive means that, in principle, these equations can be solved. Pierre-Simon Laplace was following this principle when he introduced a hypothetical daemon familiar with the Newtonian equations of motion and all the initial conditions of all the elements of a large system (the universe) and thus able to solve all equations. This daemon could then predict everything. The problem, however, is that such a daemon is hard to find. In fact, these equations can be difficult, even impossible, to solve. Already for three bodies that exert a gravitational force on each other, the famous three-body problem (e.g. Sun, Earth, Moon), there is no general analytical solution provided by algebraic and transcendental functions. This was first demonstrated by Henri Poincaré and paved the way for what is today called chaos theory. In fact, the strict Newton–Laplace program of a predictable world in terms of unambiguously computable trajectories is completely useless for most systems composed of many particles. Are these large systems not then predictable? What about systems with an extremely large number of elements, such as gases, which contain of the order of  $\mathcal{O}(10^{23})$  molecules?

Imagine that we perform the following experiment over and over again: we heat and cool water. We gain the insight that if we cool water to  $0^\circ\text{C}$  and below, it will freeze, that if we heat it to  $100^\circ\text{C}$  it will start to boil and, under standard conditions, ultimately evaporate. These phase transitions will happen with certainty. In that sense, they are predictable. We cannot predict from the equations of motion which molecule will be the first to leave the liquid. Given appropriate instrumentation, we can perhaps measure the velocity of a few single gas molecules at a point in time, but certainly not all  $10^{23}$ . What can be measured is the probability distribution that a gas molecule is observed with a specific velocity  $v$ ,

$$p(v) \sim v^2 \exp\left(-\frac{mv^2}{2kT}\right),$$

where  $T$  is temperature, and  $k$  is Boltzmann's constant. Given this probability distribution, it is possible to derive a number of properties of gases that perfectly describe their *macroscopic* behaviour and make them predictable on a macroscopic (or systemic) level.

For non-interacting particles, these predictions can be extremely precise. The predictions immediately start to degenerate as soon as there are strong interactions between the particles or if the number of particles is not large enough. Note that the term prediction now has a much weaker meaning than in the Newton–Laplace program. The meaning has shifted from being a description based on the exact knowledge of each component of a system to one based on a probabilistic knowledge of the system. Even though one can still make extremely precise predictions about multiparticle systems in a probabilistic framework, the concept of determinism is now diluted. The framework for predictions on a macroscopic level about systems composed of many particles on a probabilistic basis is called statistical mechanics.

### 1.2.3 Statistical mechanics—predictability on stochastic grounds

The aim of statistical mechanics is to understand the macroscopic properties of a system on the basis of a statistical description of its microscopic components. The idea behind it is to link the microscopic world of components with the macroscopic properties of the aggregate system. An essential concept that makes this link possible is Boltzmann–Gibbs entropy.

A system is often prepared in a macrostate, which means that aggregate properties like the temperature or pressure of a gas are known. There are typically many possible microstates that are associated with that macrostate. A microstate is a possible microscopic configuration of a system. For example, a particular microstate is one for which all positions and velocities of gas molecules in a container are known. There are usually many microstates that can lead to one and the same macrostate; for example, the temperature and pressure in the container. In statistical mechanics, the main task is to compute the probabilities for the many microstates that lead to that single macrostate. In physics, the macroscopic description is often relatively simple. Macroscopic properties are often strongly determined by the phase in which the system is. Physical systems often have very few phases—typically solid, gaseous, or liquid.

Within the Newton–Laplace framework, traditional physics works with extreme precision for very few particles or for extremely many non-interacting particles, where the statistical mechanics of Boltzmann–Gibbs applies. In other words, the class of systems that can be understood with traditional physics is not that big. Most systems are composed of many strongly interacting particles. Often, the interactions are of multiple types, are non-linear, and vary over time. Very often, such systems are complex systems.

### 1.2.4 The evolution of the concept of predictability in physics

The concept of prediction and predictability has changed in significant ways over the past three centuries. Prediction in the eighteenth century was quite different from the concept of prediction in the twenty-first. The concept of determinism has undergone at least three transitions [300].

In the *classical mechanics* of the eighteenth and nineteenth centuries, prediction meant the exact prediction of trajectories. Equations of motion would make exact statements about the future evolution of simple dynamical systems. The extension to more than two bodies has been causing problems since the very beginning of Newtonian physics; see, for example, the famous conflict between Isaac Newton and John Flamsteed on the predictability of the orbit of the Moon. By about 1900, when interest in understanding many-body systems arose, the problem became apparent. The theory of Ludwig Boltzmann, referred to nowadays as statistical mechanics, was effectively based on the then speculative existence of atoms and molecules, and it drastically changed the classical concept of predictability.

In *statistical mechanics*, based on the assumption that atoms and molecules follow Newtonian trajectories, the law of large numbers allows stochastic predictions to be made about the macroscopic behaviour of gases. Statistical mechanics is a theory of the macroscopic or collective behaviour of non-interacting particles. The concepts of predictability and determinism were subject to further change in the 1920s with the emergence of quantum mechanics and non-linear dynamics.

In *quantum mechanics*, the concept of determinism disappears altogether due to the fundamental simultaneous unpredictability of the position and momentum of the (sub-)atomic components of a system. However, quantum mechanics still allows us to make extremely high-quality predictions on a collective basis. Collective phenomena remain predictable to a large extent on a macro- or systemic level.

In *non-linear systems*, it became clear that even in systems for which the equations of motion can be solved in principle, the sensitivity to initial conditions can be so enormous that the concept of predictability must, for all practical purposes, be abandoned. A further crisis in terms of predictability arose in the 1990s, when interest in more general forms of interactions began to appear.

In *complex systems*, the situation is even more difficult than in quantum mechanics, where there is uncertainty about the components, but not about its interactions. For many complex systems, not only can components be unpredictable, but the interactions between components can also become specific, time-dependent, non-linear, and unpredictable. However, there is still hope that probabilistic predictions about the dynamics and the collective properties of complex systems are possible. Progress in the science of complex systems will, however, be impossible without a detailed understanding of the dynamics of how elements specifically interact with each other. This is, of course, only possible with massive computational effort and comprehensive data.

### 1.2.5 Physics is analytic, complex systems are algorithmic

Physics largely follows an *analytical* paradigm. Knowledge of phenomena is expressed in analytical equations that allow us to make predictions. This is possible because interactions are homogeneous, isotropic, and of a single type. Interactions in physics typically do not change over time. They are usually given and fixed. The task is to work out specific solutions regarding the evolution of the system for a given set of initial and boundary conditions.

This is radically different for complex systems, where interactions themselves can change over time as a consequence of the dynamics of the system. In that sense, complex systems change their internal interaction structure as they evolve. Systems that change their internal structure dynamically can be viewed as *machines* that change their internal structure as they operate. However, a description of the operation of a machine using analytical equations would not be efficient. Indeed, to describe a steam engine by seeking the corresponding equations of motion for all its parts would be highly inefficient. Machines are best described as *algorithms*—a list of rules regarding how the dynamics of the system updates its states and future interactions, which then lead to new constraints on the dynamics at the next time step. First, pressure builds up here, then a valve opens there, vapour pushes this piston, then this valve closes and opens another one, driving the piston back, and so on.

Algorithmic descriptions describe not only the evolution of the states of the components of a system, but also the evolution of its internal states (interactions) that will determine the next update of the states at the next time step. Many complex systems work in this way: states of components and the interactions between them are simultaneously updated, which can lead to the tremendous mathematical difficulties that make complex systems so hard to understand. These difficulties in their various forms will be addressed time and again in this book. Whenever it is possible to ignore the changes in the interactions in a dynamical system, analytic descriptions become meaningful.

Physics is generally analytic, complex systems are algorithmic. Quantitative predictions that can be tested experimentally can be made within the analytic or the algorithmic paradigm.

### 1.2.6 What are complex systems from a physics point of view?

From a physics point of view, one could try to characterize complex systems by the following extensions to physics.

- Complex systems are composed of many elements, components, or particles. These elements are typically described by their state, such as velocity, position, age, spin, colour, wealth, mass, shape, and so on. Elements may have stochastic components.
- Elements are not limited to physical forms of matter; anything that can interact and be described by states can be seen as generalized matter.
- Interactions between elements may be specific. Who interacts with whom, when, in what form, and how strong is described by interaction networks.
- Interactions are not limited to the four fundamental forces, but can be of a more complicated type. Generalized interactions are not limited to the exchange of gauge bosons, but can be mediated through exchange of messages, objects, gifts, information, even bullets, and so on.

*continued*

- Complex systems may involve superpositions of interactions of similar strengths.
- Complex systems are often chaotic in the sense that they depend strongly on the initial conditions and details of the system. Update equations that algorithmically describe the dynamics are often non-linear.
- Complex systems are often driven systems. Some obey conservation laws, some do not.
- Complex systems can exhibit a rich phase structure and have a huge variety of macrostates that often cannot be inferred from the properties of the elements. This is sometimes referred to as *emergence*. Simple forms of emergence are, of course, already present in physics. The spectrum of the hydrogen atom or the liquid phase of water are emergent properties of the involved particles and their interactions.

With these extensions, we can derive a physics-based definition for what the theory of complex systems is.

The theory of complex systems is the quantitative, predictive and experimentally testable science of generalized matter interacting through generalized interactions.

Generalized interactions are described by the interaction type and who interacts with whom at what time and at what strength. If there are more than two interacting elements involved, interactions can be conveniently described by time-dependent networks,

$$M_{ij}^{\alpha}(t),$$

where  $i$  and  $j$  label the elements in the system, and  $\alpha$  denotes the interaction type.  $M_{ij}^{\alpha}(t)$  are matrix elements of a structure with three indices. The value  $M_{ij}^{\alpha}(t)$  indicates the strength of the interaction of type  $\alpha$  between element  $i$  and  $j$  at time  $t$ .  $M_{ij}^{\alpha}(t)=0$  means no interaction of that type. Interactions in complex systems remain based on the concept of exchange; however, they are not limited to the exchange of gauge bosons. In complex systems, interactions can happen through communication, where messages are exchanged, through trade where goods and services are exchanged, through friendships, where bottles of wine are exchanged, and through hostility, where insults and bullets are exchanged.

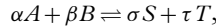
Because of more specific and time-varying interactions and the increased variety of types of interaction, the variety of macroscopic states and systemic properties increases drastically in complex systems. This diversity increase of macrostates and phenomena emerges from the properties both of the system's components and its interactions. The phenomenon of collective properties arising that are, a priori, unexpected from the elements alone is sometimes called *emergence*. This is mainly a consequence of the presence of generalized interactions. Systems with time-varying generalized interactions can exhibit an extremely rich phase structure and may be adaptive. Phases may co-exist in particular complex systems. The plurality of macrostates in a system leads to new types



of questions that can be addressed, such as: what is the number of macrostates? What are their co-occurrence rates? What are the typical sequences of occurrence? What are the life-times of macrostates? What are the probabilities of transition between macrostates? As yet, there are no general answers to these questions, and they remain a challenge for the theory of complex systems. For many complex systems, the framework of physics is incomplete. Some of the missing concepts are those of non-equilibrium, evolution, and co-evolution. These concepts will be illustrated in the sections that follow.

### 1.2.7 A note on chemistry—the science of equilibria

In chemistry, interactions between atoms and molecules are specific in the sense that not every molecule binds to (interacts with) any other molecule. So why is chemistry usually not considered to be a candidate for a theory of complex systems? To a large extent, chemistry is based on the law of mass action. Many particles interact in ways that lead to equilibrium states. For example, consider two substances  $A$  and  $B$  that undergo a reaction to form substances  $S$  and  $T$ ,



where  $\alpha, \beta, \sigma, \tau$  are the stoichiometric constants, and  $k_+$  and  $k_-$  are the forward and backward reaction rates, respectively. The forward reaction happens at a rate that is proportional to  $k_+ \{A\}^\alpha \{B\}^\beta$ , the backward reaction is proportional to  $k_- \{S\}^\sigma \{T\}^\tau$ . The brackets indicate the active (reacting) masses of the substances. Equilibrium is attained if the ratio of the reaction rates equals a constant  $K$ ,

$$K = \frac{k_+}{k_-} = \frac{\{S\}^\sigma \{T\}^\tau}{\{A\}^\alpha \{B\}^\beta}.$$

Note that the solution to this equation gives the stationary concentrations of the various substances. Technically, these equations are fixed point equations. In contrast to chemical reactions and statistical mechanics, many complex systems are characterized by being out-of-equilibrium. Complex systems are often so-called driven systems, where the system is (exogenously) driven away from its equilibrium states. If there is no equilibrium, there is no way of using fixed-point-type equations to solve the problems. The mathematical difficulties in dealing with out-of-equilibrium or non-equilibrium systems are tremendous and generally beyond analytical reach. One way that offers a handle on understanding driven out-of-equilibrium systems is the concept of self-organized criticality, which allows essential elements of the statistics of complex systems to be understood; in particular, the omnipresence of power laws.

Many complex systems are driven systems and are out-of-equilibrium.

By comparing the nature of complex systems and basic equilibrium chemistry, we learn that the mere presence of specific interactions does not automatically lead us to complex systems. However, cyclical catalytic chemical reactions [22, 113, 205], are classic prototypes of complex systems.

### 1.3 Components from the life sciences

We now present several key features of complex systems that have been adopted from biology. In particular, we discuss the concepts of evolution, adaptation, self-organization, and, again, networks.

The life sciences describe the experimental science of living matter. What is living matter? A reasonable minimal answer has been attempted by the following three statements [223]:

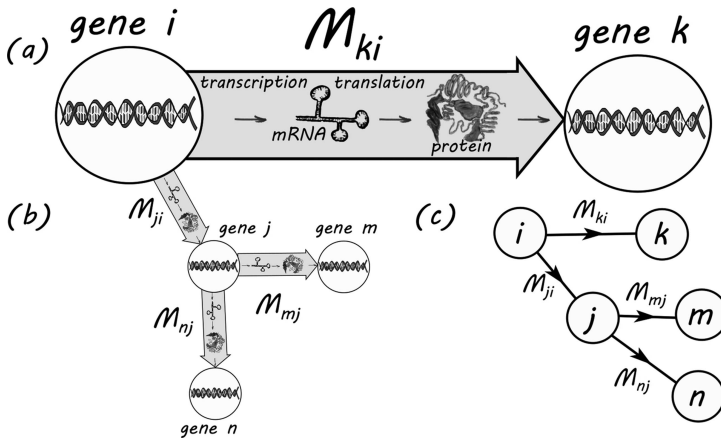
- Living matter must be self-replicating.
- It must run through at least one Carnot cycle.
- It must be localized.

Life without self-replication is not sustainable. It is, of course, conceivable that non-self-replicating organisms can be created that live for a time and then vanish and have to be recreated. However, this is not how we experience life on the planet, which is basically a single, continuous, living germ line that originated about 3.5 billion years ago, and has existed ever since. A Carnot cycle is a thermodynamic cyclical process that converts thermal energy into work, or vice versa. Starting from an initial state, after the cycle is completed, the system returns to the same initial state. The notion that living matter must perform at least one Carnot cycle is motivated by the fact that all living organisms use energy gradients (usually thermal) to perform work of some kind. For example, this work could be used for moving or copying DNA molecules. This view also pays tribute to the fact that all living objects are out-of-equilibrium and constantly driven by energy gradients. If, after performing work, a system were not able to reach its previous states, it would be hard to call it a living system. Both self-replication and Carnot cycles require some sort of localization. On this planet, this localization typically happens at the level of cells.

Living matter uses energy and performs work on short timescales without significantly transforming itself. It is constantly driven by energy gradients and is out-of-equilibrium. Self-replication and Carnot cycles require localization.

#### 1.3.1 Chemistry of small systems

Living matter, as we know it on this planet, is a self-sustained sequence of genetic activity over time. By genetic activity we mean that genes (locations on the DNA) can be turned



**Figure 1.1** Schematic view of genetic activity and what a link  $M_{ki}$  means in a genetic regulatory network. (a) Gene  $i$  activates gene  $k$  if something like the following process takes place: the activity of gene  $i$  means that a specific sub-sequence of the deoxyribonucleic acid (DNA) (gene) is copied into a complementary structure, an mRNA molecule. This mRNA molecule from gene  $i$ , might get ‘translated’ (copied again) into a protein of type  $i$ . This protein can bind with other proteins to form a cluster of proteins, a ‘complex’. Such complexes can bind to other regions of the DNA, say, the region that is associated with gene  $k$ , and thereby cause the activation of gene  $k$ . (b) Gene  $i$  causes gene  $j$  to become active, which activates genes  $m$  and  $n$ . (c) The process, where the activity of gene  $i$  triggers the activity of other genes, can be represented as a directed genetic regulatory network. Complexes can also deactivate genes. If gene  $j$  is active, a complex might deactivate it.

‘on’ and ‘off’. If a gene is on, it triggers the production of molecular material, such as ribonucleic acid (RNA) that can later be translated into proteins. A gene is typically turned on by a cluster of proteins that bind to each other to form a so-called ‘complex’. If such a cluster binds to a specific location on the DNA, this could cause a copying process to be activated at this position; the gene is then active or ‘on’; see Figure 1.1.

Genetic activity is based on chemical reactions that take place locally, usually within cells or their nuclei. However, these chemical reactions are special in the sense that only a few molecules are involved [341]. In traditional chemistry, reactions usually involve billions of atoms or molecules. What happens within a cell is chemistry with a *few* molecules. This immediately leads to a number of problems:

- It can no longer be assumed that molecules meet by chance to react.
- With only a few molecules present that might never meet to react, the concept of equilibrium becomes useless.
- Without equilibrium, there is no law of mass action.

If there is no law of mass action, how can chemistry be done? Classical equilibrium chemistry is inadequate for dealing with molecular mechanisms in living matter. In cells, molecules are often actively transported from the site of production (typically, the nucleus, for organisms that have one) to where they are needed in the cell. This means that diffusion of molecules no longer follows the classical diffusion equation. Instead, molecular transport is often describable by an anomalous diffusion equation of the form,

$$\frac{d}{dt}p(x,t) = D \frac{d^{2+\nu}}{dx^{2+\nu}}p(x,t)^\mu,$$

where  $p(x,t)$  is the probability of finding a molecule at position  $x$  at time  $t$ ,  $D$  is the diffusion constant, and  $\mu$  and  $\nu$  are exponents that make the diffusion equation non-linear.

Chemical binding often depends on the three-dimensional structure of the molecules involved. This structure can depend on the ‘state’ of the molecules. For example, a molecule can be in a normal or a phosphorylated state. Phosphorylation happens through the addition of a phosphoryl group ( $\text{PO}_3^{2-}$ ) to a molecule, which may change its entire structure. This means that for a particular state of a molecule it binds to others, but does not bind if it is in the other state. A further complication in the chemistry of a few particles arises with the reaction rates. By definition, the term reaction rate only makes sense for sufficiently large systems. The speed of reactions depends crucially on the statistical mechanics of the underlying small system and fluctuation theorems may now become important [122].

### 1.3.2 Biological interactions happen on networks—almost exclusively

Genetic regulation governs the temporal sequence of the abundance of proteins, nucleic material, and metabolites within any living organism. To a large extent, genetic regulation can be viewed as a discrete interaction: a gene is active or inactive; a protein binds to another or it does not; a molecule is phosphorylated or not. Discrete interactions are well-described by networks. In the context of the life sciences, three well-known networks are the metabolic network, the protein–protein binding network, and the Boolean gene-regulatory network. The metabolic network<sup>1</sup> is the set of linked chemical reactions occurring within a cell that determine the cell’s physiological and biochemical properties. The metabolic network is often represented in networks of chemical reactions, where nodes represent substances and directed links (arrows) correspond to reactions or catalytic influences. The protein–protein networks represent empirical findings about protein–protein interactions (binding) in network representations [102]. Nodes are proteins, and links specify the interaction type between them. Different interaction types include stable, transient, and homo- or hetero-oligomer interactions.

<sup>1</sup> For an example of what metabolic networks look like, see <http://biochemical-pathways.com/#!/map/1>

### 1.3.3 What is evolution?

‘Nothing in biology makes sense except in the light of evolution’. Theodosius Dobzhansky

Evolution is a natural phenomenon. It is a process that increases and destroys diversity, and it looks like both a ‘creative’ and a ‘destructive’ process. Evolution appears in biological, technological, economical, financial, historical, and other contexts. In that sense, evolutionary dynamics is universal. Evolutionary systems follow characteristic dynamical and statistical patterns, regardless of the context. These patterns are surprisingly robust and, as a natural phenomenon, they deserve a quantitative and predictive scientific explanation.

What is evolution? Genetic material and the process of replication involve several stochastic components that may lead to variations in the offspring. Replication and variation are two of the three main ingredients of evolutionary processes. What evolution means in a biological context is captured by the classic Darwinian narrative. Consider a population of some kind that is able to produce offspring. This offspring has some random variations (e.g. mutations). Individuals with the optimal variations with respect to a given environment have a selection advantage (i.e. higher fitness). Fitness manifests itself by higher reproductive success. Individuals with optimal variations will have more offspring and will thus pass their particular variations on to a new generation. In this way ‘optimal’ variations are selected over time. This is certainly a convincing description of what is going on; however, in this form it may not be useful for predictive science. How can we predict the fitness of individuals in future generations, given that life in future environments will look very different from what it is today? Except over very short time periods, this is a truly challenging task that is far from understood. There is a good prospect, however, of the *statistics* of evolutionary systems being understood. The Darwinian scenario fails to explain essential features about evolutionary systems, such as the existence of boom and crash phases, where the diversity of systems radically changes within short periods of time. An example is the massive diversification (explosion) of species and genera about 500 million years ago in the Cambrian era. It will almost certainly never be possible to predict what species will live on Earth even 500 years from now, but it may be perfectly possible to understand the statistics of evolutionary events and the factors that determine the statistics. In particular, statistical statements about expected diversity, diversification rates, robustness, resilience, and adaptability are coming within reach. In Chapter 5 we will discuss approaches to formulating evolutionary dynamics in ways that make them accessible both combinatorially and statistically.

The concept of evolution is not limited to biology. In the economy, the equivalent of biological evolution is innovation, where new goods and services are constantly being produced by combination of existing goods and services. Some new goods will be selected in markets, while the majority of novelties will not be viable and will vanish. The industrial revolution can be seen as one result of evolutionary dynamics, leading, as it did, to an ongoing explosion of diversification of goods, services, and innovations.

Another example of evolutionary dynamics outside biology is the sequence of invention and discovery of chemical compounds. The history of humankind itself is an example of evolutionary dynamics. Evolutionary dynamics can take place simultaneously at various scales. In biological settings, it works at the level of molecules, cells, organisms, and populations; in economic settings, it can work at product, firm, corporation, and country level. A famous application of evolutionary dynamics in computer science are so-called genetic algorithms [194]. These algorithms mimic natural selection by iteratively producing copies of computer code with slight variations. Those copies that perform best for a given problem (usually an optimization task) are iteratively selected and are passed onto the next ‘generation’ of codes.

### **1.3.3.1 Evolution is not physics**

To illustrate that evolution is not a process that can be described with traditional physics, we define an evolutionary process as a three-step process:

1. A new thing comes into existence within a given *environment*.
2. The new thing has the chance to interact with its environment. The result of this interaction is that it gets ‘selected’ (survives) or is destroyed.
3. If the new thing gets selected in the environment, it becomes part of this environment (boundary) and thus transforms the old environment into a new one. New and arriving things in the future will experience the new environment. In that sense, evolution is an algorithmic process that co-evolves its boundaries.

If we try to interpret this three-step process in terms of physics, we immediately see that even if we were able to write down the dynamics of the system in the form of equations of motion, we would not be able to fix the system’s boundary conditions. Obviously, the environment plays the role of the boundary conditions within which the interactions happen. The boundary conditions evolve as a consequence of the dynamics of the system and change at every instant. The dynamics of the boundary conditions is dynamically coupled with the equations of motion. Consequently, as the boundary conditions cannot be fixed, this set of equations cannot, in general, be solved and the Newtonian method breaks down. A system of dynamical equations that are coupled dynamically to their boundary conditions is a mathematical monster. That is why an algorithmic process like evolution is hard to solve using analytical approaches.<sup>2</sup>

The second problem associated with evolutionary dynamics, from a physics point of view, is that the phasespace is not well-defined. As new elements may arrive at any point in time, it is impossible to prestate what the phasespace of such systems will be. Obviously, this poses problems in terms of producing statistics with these systems. The situation could be compared to trying to produce statistics by rolling a dice, whose number of faces changes from one throw to the next.

<sup>2</sup> Such systems can be treated analytically whenever the characteristic timescales of the processes involved are different. In our example, this would be the case if the dynamics of the interactions of the ‘new thing’ with the environment happens on a fast timescale, while changes in the environment happen slowly.

Evolutionary dynamics is radically different from physics for two main reasons:

- In evolutionary systems, boundary conditions cannot be fixed.
- In evolutionary systems, the phasespace is not well defined—it changes over time. New elements may emerge that change the environment and therefore also the dynamics for all the existing elements of the system.

Evolutionary aspects are essential for many complex systems and cannot be ignored. A great challenge in the theory of complex systems is to develop a consistent framework that is nevertheless able to deal with evolutionary processes in quantitative and predictive terms. We will see how a number of recently developed mathematical methods can be used to address and deal with these two fundamental problems. In particular, in Chapter 5, we will discuss combinatorial evolution models. These models are a good example of how algorithmic approaches lead to quantitative and testable predictions.

### 1.3.3.2 *The concept of the adjacent possible*

A helpful steppingstone in addressing the problem of dynamically changing phasespaces is the concept of the *adjacent possible*, proposed by Stuart Kauffman [223]. The adjacent possible is the set of all possible states of the world that *could* potentially exist in the next time step, given the present state of the world. It drastically reduces the size of phasespace from all possible states to a set of possibilities that are conditional on the present. Obviously, not everything can be produced within the next time step. There are many states that are impossible to imagine, as the components required to make them do not yet exist. In other words, the adjacent possible is the subset of all possible worlds that are *reachable* within the next time step and depends strongly on the present state of the world. In this view, evolution is a process that continuously ‘fills’ its adjacent possible. The concrete realization of the adjacent possible at one time step determines the adjacent possible at the next time step.

Thus, in the context of biological evolution or technological innovation, the adjacent possible is a huge set, in which the present state of the world determines the potential realization of a vast number of possibilities in the next time step. Typically, the future states are not known. In contrast, in physics, a given state often determines the next state with high precision. This means that the adjacent possible is a very small set. For example, the adjacent possible of a falling stone is given by the next position (point) on its parabolic trajectory. In comparison, the adjacent possible of an ecosystem consists of all organisms that can be born within the next time step, with all possible mutations and variations that can possibly happen—a large set of possibilities indeed. The concept of the adjacent possible introduces path-dependence in the stochastic dynamics of phasespace. We will discuss the statistics of path-dependent evolutionary processes in Chapters 5 and 6.

### 1.3.3.3 *Summary evolutionary processes*

Evolutionary processes are relevant to the treatment of complex systems for the following reasons.

- For evolutionary systems, boundary conditions cannot usually be fixed. This means that it is impossible to take the system apart and separate it from its context without massively altering and perhaps even destroying it. The concept of reductionism is inadequate for describing evolutionary processes.
- Evolutionary complex systems change their boundary conditions as they unfold in time. They co-evolve with their boundary conditions. Frequently, situations are difficult or impossible to solve analytically.
- For complex systems, the adjacent possible is a large set of possibilities. For physics, it is typically a very small set.
- The adjacent possible itself evolves.
- In many physical systems, the realization of the adjacent possible does not influence the next adjacent possible; in evolutionary systems, it does.

### 1.3.4 Adaptive and robust—the concept of the edge of chaos

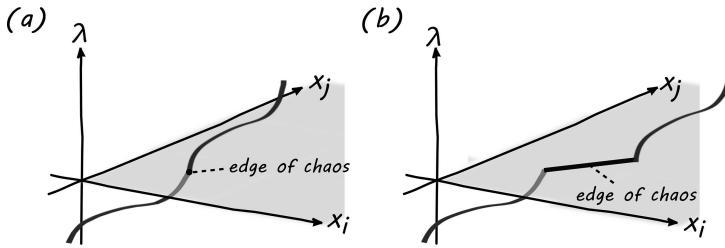
Many complex systems are robust and adaptive at the same time. The ability to adapt to changing environments and to be robust against changing environments seem to be mutually exclusive. However, most living systems are clearly adaptive and robust at the same time. As an explanation for how these seemingly contradictory features could co-exist, the following view of the *edge of chaos* was proposed [246]. Every dynamical system has a maximal Lyapunov exponent, which measures how fast two initially infinitesimally close trajectories diverge over time. The exponential rate of divergence is the Lyapunov exponent,  $\lambda$ ,

$$|\delta X(t)| \sim e^{\lambda t} |\delta X(0)|,$$

where  $|\delta X(t)|$  is the distance between the trajectories at time  $t$  and  $|\delta X(0)|$  is the initial separation. If  $\lambda$  is positive, the system is called *chaotic* or strongly mixing. If  $\lambda$  is negative, the system approaches an attractor, meaning that two initially infinitesimally separated trajectories converge. This attractor can be a trivial point (fixed point), a line (limit cycle), or a fractal object. An interesting case arises when the exponent  $\lambda$  is exactly zero. The system is then called quasi-periodic or at the ‘edge of chaos’. There are many low-dimensional examples where systems exhibit all three possibilities—they can be chaotic, periodic, or at the edge of chaos, depending on their control parameters. The simplest of these is the logistic map.

The intuitive understanding of how a system can be adaptive and robust at the same time if it operates at the edge of chaos, is given by the following. If  $\lambda$  is close to zero, it takes only tiny changes in the system to move it from a stable and periodic mode ( $\lambda$  slightly negative) to the chaotic phase ( $\lambda$  positive). In the periodic mode, the system is stable and robust; it returns to the attractor when perturbed. When it transits into the chaotic phase, say, through a strong perturbation in the environment, it will sample large regions



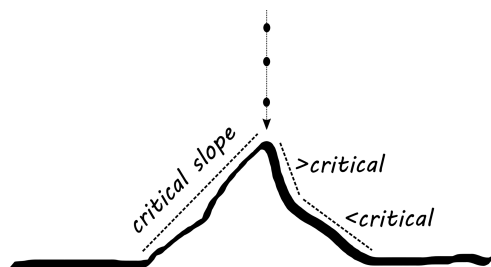


**Figure 1.2** Schematic view of the edge of chaos. (a) Shows the largest Lyapunov exponent in the parameter space (indicated by  $x_i$  and  $x_j$ ) of a dynamical system. The largest exponent dominates the dynamics of the system. For every point in parameter space, the Lyapunov exponent is either positive (chaotic), negative (periodic), or exactly zero—which means at the ‘edge of chaos’. The edge of chaos offers a pictorial understanding of how systems can be adaptive and robust at the same time. Systems at the edge of chaos can be thought of as being usually just inside the regular regime. They can transit to the chaotic region very quickly. Once in the chaotic regime, vast volumes of phasespace can be explored which possibly contain regions that are ‘better’ for the system. Once such a region is found, the system can transit back to the periodic region. Note that the region of parameter space where the Lyapunov exponent is zero is tiny. Some evolutionary complex systems show that this region can be drastically inflated. This will be discussed in Chapter 5. (b) Shows a situation for an inflated edge of chaos.

of phasespace very quickly. By sampling large volumes of phasespace, the system has the chance to find new ‘solutions’ that are compatible with the perturbed environment and can then again settle into a periodic phase. The system adapted by sampling other optima. This situation is comparable to a simulated annealing procedure in a computer code.

#### 1.3.4.1 How does nature find the edge of chaos?

For many non-linear dynamical systems, the set of points at which the Lyapunov exponents are exactly zero is very limited and often of measure zero; see Figure 1.2a. If living systems operate at the edge of chaos, how did evolution find and select these points? How can a mechanism of evolution detect something that is of measure zero? One possible explanation is that the regions where the Lyapunov exponent is zero is not of measure zero, but are extended areas in parameter space. Indeed, simple evolutionary models do show inflated regions of the edge of chaos [356]; see Figure 1.2b. We discuss situations where this possibility seems to be realized in Chapter 5. Another explanation is self-organized criticality. This is a mechanism that allows systems to endogenously organize themselves to operate at a critical point that separates the chaotic from the regular regime [24, 226]. A critical point in physics is a point in parameter space where a system is at a phase transition point. These points are reached at conditions (temperature, pressure, slope in a sand pile, etc.) where characteristic quantities (e.g. correlation length) become divergent. Think, for example, of the critical temperature at which a magnetization transition occurs, the Curie temperature  $T_c$ . Above that temperature there is no magnetization. Approaching the Curie temperature shows that, at the critical



**Figure 1.3** Sand pile models are models for self-organized criticality. These systems self-organize towards a critical state, which is characterized by the fact that the system develops dynamics that are felt across the entire system; in other words, it develops diverging correlation lengths. In sand piles, the system organizes towards a critical slope, above which avalanches of sand will occur to reduce the slope and below which sand is deposited close to the sites where the sand hits, which makes the slope steeper. The size distribution of avalanches is a power law, meaning that it covers a large spectrum of sizes. The frequency distribution of the occurrence of avalanches is also a power law. Besides being a playground for understanding self-organized criticality, sand pile models have practical applications in the science of earthquakes and collapse.

point, quantities, such as the magnetic susceptibility  $\chi$  start to diverge as a power law,  $\chi = (T - T_c)^{-\gamma}$ , where  $\gamma$  is a critical exponent. In many physical systems, these transition points are unique and parameters have to be fine-tuned to these critical points to find the power law behaviour. Self-organized critical systems manage to find these critical points endogenously, without any fine-tuning. Self-organized criticality seems to be realized in a wide range of systems, including sand piles, precipitation, heartbeats, avalanches, forest fires, earthquakes, financial markets, combinatorial evolution, and so on. It often occurs in slowly driven systems, where driven means that they are driven away from equilibrium.

Self-organized critical systems are dynamical, out-of-equilibrium systems that have a critical point as an attractor. These systems are characterized by (approximate) scale invariance or ‘scaling’. Scale invariance means the absence of characteristic scales, and it often manifests itself in the form of power laws in the associated probability distribution functions. Self-organized criticality is one of the classic ways of understanding the origin of power laws, which are omnipresent in complex systems. Other ways of understanding power laws include criticality, multiplicative processes with constraints, preferential dynamics, extremal optimization methods, and sample space reducing processes. We will discuss the mechanisms for understanding the origin of power laws in Chapter 3.

#### 1.3.4.2 Intuition behind self-organized critical systems—sand pile models

Imagine sand is dropped onto a table as shown in Figure 1.3. A pile gradually builds up. If you consider the slopes of the pile, you will observe that they are not constant but that they vary in terms of their slope angles. If the slope becomes too steep, avalanches go off and the slope becomes flatter again. If the slope is flat, sand becomes deposited and the slope becomes steeper. In other words, the pile *self-organizes* itself towards a critical slope. The system is robust and adaptive.

### 1.3.5 Components taken from the life sciences

Let us now put together the components we need for a description of complex systems adapted from the life sciences.

- Interactions between elements happen specifically. They take place on networks. Often, interactions are discrete; they either happen or not. Often, systems operate algorithmically.
- Complex systems are out-of-equilibrium, which makes them hard to deal with analytically. If they are self-organized critical, the statistics behind them can be understood.
- Many complex systems follow evolutionary dynamics. As they progress, they change their own environment, their context, or their boundary conditions.
- Many complex systems are adaptive and robust at the same time. They operate at the ‘edge of chaos’. Self-organized criticality is a mechanism that regulates systems towards their edge of chaos.
- Most evolutionary complex systems are path-dependent and have memory. They are therefore non-ergodic and non-Markovian. The adjacent possible is a way of conceptualizing the evolution of the ‘reachable’ phasespace.

## 1.4 Components from the social sciences

Social science is the science of social interactions and their implications for society.

Usually, social science is neither very quantitative or predictive, nor does it produce experimentally testable predictions. It is largely qualitative and descriptive. This is because, until recently, there was a tremendous shortage of data that are both time-resolved (longitudinal) and multidimensional. The situation is changing fast with the new tendency of *homo sapiens* to leave electronic fingerprints in practically all dimensions of life. The centuries-old data problem of the social sciences is rapidly disappearing. Another fundamental problem in the social sciences is the lack of reproducibility or

repeatability. On many occasions, an event takes place once in history and no repeats are possible.

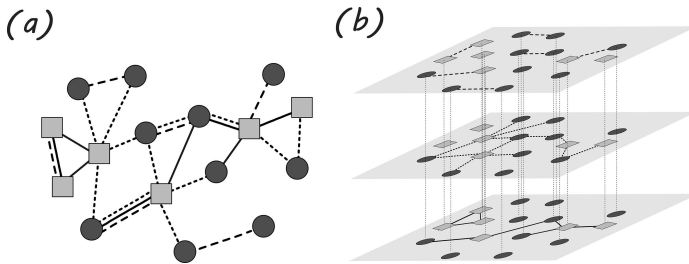
As in biology, social processes are hard to understand mathematically because they are evolutionary, path-dependent, out-of-equilibrium, and context-dependent. They are high-dimensional and involve interactions on multiple levels. The methodological tools used by traditional social scientists have too many shortcomings to address these issues appropriately. Unfortunately, the tools of social science practised today rarely extend much beyond linear regression models, basic statistics, and game theory. In some branches of social science, such as economics, there is a tradition of ignoring the scientific principle in the sense that data, even if they are available, are not taken seriously. There are influential ‘theories’ that are in plain contrast to experimental evidence, including the capital asset pricing model, the efficient market hypothesis, or the Markowitz portfolio theory. These concepts earned their inventors Nobel Prizes. What did also not occur to date in the social sciences are the massive joint and coordinated efforts between scientists that have been taking place in physics (CERN), biology (the genome project), and climate science. However, two important components have been developed in the social sciences and play a crucial role in the theory of complex systems:

- *Multilayer interaction networks.* In social systems, interactions happen simultaneously at more or less the same strength scale on a multitude of superimposed interaction networks. Social scientists, in particular sociologists, have recognized the importance of social networks<sup>3</sup> since the 1970s [156, 398].
- *Game theory.* Another contribution from the social sciences, game theory, is a concept that allows us to determine the outcome of rational interactions between agents trying to optimize their payoff or utility [393]. Each agent is aware that the other agent is rational and that he/she also knows that the other agent is rational. Before computers arrived on the scene, game theory was one of the very few methods of dealing with complex systems mathematically. Game theory can easily be transferred to dynamical situations, and it was believed for a long time that iterative game-theoretic interactions were a way of understanding the origin of cooperation in societies. This view is now severely challenged by the discovery of so-called zero-determinant games [316]. Game theory was first developed and used in economics but has penetrated other fields of the social and behavioural sciences.

### 1.4.1 Social systems are continuously restructuring networks

Social systems can be thought of as time-varying multilayer (multiplex) networks. Nodes are individuals or institutions, and links are interactions of different types. Interactions

<sup>3</sup> Interestingly, until very recently, networks were not recognized as relevant by the ‘queen’ of the social sciences, economics, even though networks clearly dominate practically every domain of the economy. Mainstream economics has successfully ignored networks—production networks, distribution networks, trading and consumption networks, ownership networks, information networks, and financial networks—for more than a century in favour of a rather unrealistic equilibrium view of the economy.



**Figure 1.4** Two schematic representations of the same multilayer network. Nodes are characterized by a two-dimensional state vector. The first component is given by colours (light- and dark-grey) the second by shapes (circles, squares). Nodes interact through three types of interaction that are represented by (full, broken, and dotted) lines. (a) Shows the projection of the multilayer network to a single layer, whereas in (b) each type of link is shown in a different layer. The system is complex if states simultaneously change as a function of the interaction network and if interactions change as a function of the states; see Equation 1.1. The multilayer network could represent a network of banks at a given moment, where shapes represent the wealth of the bank and the links could represent financial assets that connect banks with each other. A full line could mean a credit relation; a broken line could represent derivatives trading, and dotted lines indicate if one bank owns shares in another bank. Depending on that network, the banks will make a profit or loss in the next time step.

change over time. The types of link can be friendship, family ties, exchange of goods, payments, trust, communication, enmity, and so on. Every type of link is represented by a separate network layer; see, for example, Figure 1.4. Individuals interact through a superposition of these different interaction types (multilayer network), which happen simultaneously and are often of the same order of magnitude in ‘strength’. Often, networks at one level interact with networks at other levels. Networks that characterize social systems show a rich spectrum of growth patterns and a high level of plasticity. This plasticity of networks arises from restructuring processes through link creation, relinking, and link removal. Understanding and describing the underlying restructuring dynamics can be very challenging; however, there are a few typical and recurring dynamical patterns that allow for scientific progress. We will discuss these in Chapter 4.

Individuals are characterized by states, such as their wealth, gender, education level, political opinion, age, and so on. Some of these states can dynamically change over time. States typically have an influence on the linking dynamics of the corresponding individual (node). If that is the case, a tight connection exists between network structure and node states. The joint dynamics of network restructuring and changes of states by individuals is a classic example of co-evolution.

## 1.5 What are Complex Systems?

We present a one-sentence summary of what complex systems are, which covers most of the features discussed in the previous sections:

Complex systems are co-evolving multilayer networks.

This statement summarizes the following ten facts about complex systems and provides an intuitive picture of the essence of complex systems.

1. Complex systems are composed of many elements. These are labelled with latin indices,  $i$ .
2. These elements interact with each other through one or more interaction types, labelled with greek indices,  $\alpha$ . Interactions are often specific between elements. To keep track of which elements interact, we use networks. Interactions are represented as links in the interaction networks. The interacting elements are the nodes in these networks. Every interaction type can be seen as one network layer in a multilayer network; see Figure 1.4. A multilayer network is a collection of networks linking the same set of nodes. If these networks evolve independently, multilayer networks are just superpositions of networks. However, there are often interactions between interaction layers.
3. Interactions are not static but change over time. We use the following notation to keep track of interactions in the system. The strength of an interaction of type  $\alpha$  between two elements  $i$  and  $j$  at time  $t$  is denoted by,

$$M_{ij}^{\alpha}(t).$$

Interactions can be physical, chemical, social, or symbolic. Most interactions are mediated through some sort of exchange process between nodes. In that sense, interaction strength is often related to the quantity of objects exchanged (gauge bosons for physical interactions, electrons for chemical interactions, financial assets for economical interactions, bottles of wine for positive social interactions, and bullets for aggressive ones, etc.). Interactions can be deterministic or stochastic.

4. Elements are characterized by states. States can be scalar; if an element has various independent states, it will be described by a state vector or a state tensor. States are not static but evolve with time. We denote state vectors by,

$$\sigma_i(t).$$

States can be the velocity of a planet, spin of an electron, state of phosphorylation of a protein capitalization of a bank, or the political preference of a person. State changes can be deterministic or stochastic. They can be the result of an endogenous dynamics or of external driving.

5. Complex systems are characterized by the fact that states and interactions are often not independent but evolve together by mutually influencing each other; states and interactions *co-evolve*. The way in which states and interactions are coupled can be deterministic or stochastic.

6. The dynamics of co-evolving multilayer networks is usually highly non-linear.
7. Complex systems are context-dependent. Multilayer networks provide that context and thus offer the possibility of a self-consistent description of complex systems. To be more precise, for any dynamic process happening on a given network layer, the other layers represent the ‘context’ in the sense that they provide the only other ways in which elements in the initial layer can be influenced. Multilayer networks sometimes allow complex systems to be interpreted as ‘closed systems’. Of course, they can be externally driven and usually are dissipative and non-Hamiltonian. In that sense, complex systems are hard to describe analytically.
8. Complex systems are *algorithmic*. Their algorithmic nature is a direct consequence of the discrete interactions between interaction networks and states.
9. Complex systems are path-dependent and consequently often non-ergodic. Given that the network dynamics is sufficiently slow, the networks in the various layers can be seen as a ‘memory’ that stores and records the recent dynamical past of the system.
10. Complex systems often have memory. Information about the past can be stored in nodes, if they have a memory, or in the network structure of the various layers.

In this book, we assume that a co-evolving multilayer network structure is the fundamental dynamical backbone of complex systems. This assumption not only provides a simple conceptual framework, it also allows us to explain several of the essential properties of complex systems. These include:

- the emergence and origin of power laws,
- self-organized criticality,
- collapse and boom phases in evolutionary dynamics,
- the nature of phase transitions,
- the origin of the edge of chaos,
- statistics of path-dependent processes.

A snapshot of a co-evolving multilayer network is shown in Figure 1.4. Nodes are represented by a state vector with two components, colour (light- and dark-grey) and shape (circles and boxes). Nodes interact through three types of interaction (full, broken, and dotted lines). The system is a complex system if states change as a function (deterministic or stochastic) of the interaction network and, simultaneously, interactions (the networks) change as a function of the states. See also Equations (1.1). For example, the multilayer network shown could represent a network of banks on a given day, where the shape of the nodes represents the wealth of the bank (circle indicates rich, box indicates poor) and the colour represents the gender of the CEO of the bank (light-grey is female, dark-grey is male). The links represent financial contracts (assets) between banks; a full line could mean a credit relation, a broken line could represent derivatives trading, and dotted lines could indicate that one bank owns shares in another. The set

of links associated with a bank can be seen as its portfolio. Clearly, the wealth state of a bank will influence the network structure. If a bank is poor, it is not allowed to issue new credits. At the same time, the network structure of assets (the portfolio) has a huge effect on the future wealth of the banks. On the other hand, the gender of the CEO may have little effect on the interbank network structure, and the networks will certainly not have any effect on the gender of the CEO. While the wealth-asset network is a complex system, the gender-network system is not.

### 1.5.1 What is co-evolution?

To provide some insights into what we mean by co-evolution, we formulate it in a slightly more formal way. In general, interactions can change the states of the elements. In physics, gravitational interaction changes the momentum of massive objects; electromagnetic interactions lead to spin flips; chemical interactions may change the binding state of proteins; economic interactions change the portfolios of traders; and social interactions may change sympathy levels.

The interaction partners of a node in a network (or multilayer network) can be seen as the local ‘environment’ of that node. The environment often determines the future state of the node. In complex systems, interactions can change over time. For example, people establish new friendships or economic relations; countries terminate diplomatic relations. The state of nodes determines (fully or in part) the future state of the link, whether it exists in the future or not and, if it exists, the strength and the direction that it will have.

The essence of co-evolution can be encompassed in the statement:

- The state of the network (topology and weights) determines the future states of the nodes.
- The state of the nodes determines the future state of the links of the network.

More formally, co-evolving multiplex networks can be written as,

$$\begin{aligned}\frac{d}{dt}\sigma_i(t) &\sim F\left(M_{ij}^\alpha(t), \sigma_j(t)\right) \\ \frac{d}{dt}M_{ij}^\alpha(t) &\sim G\left(M_{ij}^\beta(t), \sigma_j(t)\right).\end{aligned}\tag{1.1}$$

Here, the derivatives mean ‘change within the next time step’ and should not be confused with real derivatives. The first equation means that the states of element  $i$  change as a ‘function’,  $F$ , that depends on the present states of  $\sigma_i$  and the present multilayer network states,  $M_{ij}^\alpha(t)$ . The function  $F$  can be deterministic or stochastic and contains all summations over greek indices and all  $j$ . The first equation depicts the analytical nature of physics that has characterized the past 300 years. Once one specifies  $F$  and the initial



conditions, say,  $\sigma_i(t=0)$ , the solution of the equation provides us with the trajectories of the elements of the system. Note that in physics the interaction matrix  $M_{ij}^\alpha(t)$  represents the four forces. Usually, it only involves a single interaction type  $\alpha$ , is static, and only depends on the distance between  $i$  and  $j$ . Typically, systems that can be described with the first equation alone are not called complex, however complicated they may be.

The second equation specifies how the interactions evolve over time as a function  $G$  that depends on the same inputs, states of elements and interaction networks.  $G$  can be deterministic or stochastic. Now interactions evolve in time. In physics this is very rarely the case. The combination of both equations makes the system a co-evolving complex system. Co-evolving systems of this type are, in general, no longer analytically solvable.<sup>4</sup> One cannot solve these systems using the rationale of physics because the environment—or the boundary conditions—specified by  $M$  change as the system evolves. From a practical point of view, Equations 1.1 are useless until the functions  $G$  and  $F$  are specified. Much of the science of complex systems is related to identifying and giving meaning to these functions for a concrete system at hand. This can be done in an analytical or algorithmic way, meaning that  $F$  and  $G$  can be given by analytical expressions or algorithmic ‘update rules’. Both can be deterministic or stochastic.

More and more data sets containing full information about a system are becoming available, meaning that all state changes and all interactions between the elements are recorded. It is becoming technically and computationally possible to monitor cell-phone communication networks on a national scale, to monitor all genetic molecular activities within a cell, or all legal financial transactions on the planet. Data that contain time-resolved information on states and interactions can be used to actually visualize Equations (1.1); all the necessary components are listed in the data at any point in time: the interaction networks  $M_{ij}^\alpha$ , the states of the elements  $\sigma_i$ , and all the changes  $\frac{d}{dt}\sigma_i$  and  $\frac{d}{dt}M_{ij}^\alpha$  over time. Even though Equations (1.1) might not be analytically solvable, it is becoming possible for more and more situations to ‘watch’ them. It is often possible to formulate agent-based models of complex systems in the exact form of Equations (1.1), and this allows us to make quantitative and testable predictions.

The structure of Equations (1.1) is, of course, not the most general possible. Immediate generalizations would be to endow the multilayer networks with a second greek index,  $M_{ij}^{\alpha\beta}$ , which would allow us to capture cross-layer interactions between elements. It is conceivable that elements and interactions are embedded in space and time; indices labelling the elements and interactions could carry such additional information,  $i(x, t, \dots)$  or  $\{ij\}^{\alpha\beta}(x, t, \dots)$ . Finally, one could introduce memory to the elements and interactions of the system.

## 1.5.2 The role of the computer

The science of complex systems is unthinkable without computers. The analytical tools available until the 1980s were good enough to address problems based on differential

<sup>4</sup> Except for simple examples or situations, where the timescale of the dynamics of the states is clearly different from the dynamics of the interaction networks.

equations, for systems in equilibrium, for linear (or sufficiently linearizable) systems, and for stochastic systems with weak interactions. The problems associated with evolutionary processes, non-ergodicity, out-of-equilibrium systems, self-organization, path-dependence, and so on, were practically beyond scientific reach, mainly because of computational limits. The computational power to address these issues has only become available in the past decades.

Often, computer simulations are the only way of studying and developing insights into the dynamics of complex systems. Simulations are often referred to by agent-based models, where elements and their interactions are modelled and simulated dynamically. Agent-based models allow us to study the collective outcomes of systems comprising elements with specific properties and interactions. The algorithmic description of systems in terms of update rules for states and interactions is fully compatible with the way computer simulations are done. In many real-world situations there is only a single history and this cannot be repeated. This occurs in social systems, in the economy, or in biological evolution. Computer simulations allow us to create artificial histories that are statistically equivalent copies. Ensembles of histories can be created that help us understand the systemic properties of the systems that lead to them. Without simulations, predictive statements about systemic properties like robustness, resilience, efficiency, likelihood of collapse, and so on, would never be possible. The possibility of creating artificial histories solves the problem of repeatability.

With the current availability of computer power and high-dimensional and time-resolved data, computational limits or data issues no longer pose fundamental bottlenecks for understanding complex systems. The bottleneck for progress is the theory of complex systems, a mathematically consistent framework in which data can be systematically transformed into useful knowledge.

The computer has fundamentally changed the evolution of science. It has finally opened and paved the way to understanding complex adaptive systems as a natural science on a quantitative, predictive, and testable basis.

## 1.6 The structure of the book

Complex systems span an immense universe of phenomena, systems, and processes. We believe that most of these can be mapped, in one way or another, into the framework of the stochastic, co-evolving, multilayer networks that we sketched in Equations (1.1). To be able to treat those systems in quantitative and predictive ways, we need tools and concepts for random processes, networks, and evolutionary dynamics. These needs define the structure of the book.

Complex systems involve many different sources of randomness in their components, interactions, processes, time series, structures, and so on. In Chapter 2 we review the basic notions of randomness and statistics that will be needed in various parts of the

book. In Chapter 3 we discuss the notion of scaling and learn why it is helpful. We review the classic routes to understanding the origin of power laws, which are omnipresent in the statistical description of complex systems. One of the central backbones of complex systems are dynamical networks, which tell us how the building blocks interact with each other. Dynamics can happen on networks (e.g. diffusion on networks), or the networks dynamically rearrange themselves. The notions and basic concepts of networks, their structures, characteristics, functions, and ultimately their dynamics will be developed in Chapter 4.

Evolutionary dynamics is central to many complex adaptive systems. After reviewing classic ways of understanding the dynamics of evolutionary systems, in Chapter 5 we show how a general model of evolutionary systems can be related to co-evolving network structures. We will learn that this approach is an example of an algorithmic description of systems. We will further see that evolutionary systems have familiar phase diagrams and can be naturally associated to self-organized critical systems.

Finally, in Chapter 6 we probe how far methods from statistical mechanics, information theory, and statistical inference methods can be used in the context of stochastic complex systems. These systems are typically path-dependent, evolutionary, non-Markovian, and non-ergodic; thus, the methods that we have learned in physics, statistics, and information theory should be inapplicable. The chapter is designed to show that a careful generalization of the classic concepts of entropy, information production, and statistical inference methods also allows us to use these concepts for (simple) complex systems and for path-dependent processes in particular.

All chapters start in a relatively simple fashion and become more difficult towards the end. We conclude most chapters with extensive examples that should provide an impression of the status of actual research.

### 1.6.1 What has complexity science contributed to the history of science?

We conclude this chapter with a somewhat incomplete reading list containing several classics and a few more recent contributions from the science of complex systems. Some of them have already changed our world view:

- network theory [291],
- genetic regulatory networks [221, 222],
- Boolean networks [225],
- self-organized criticality [24, 226],
- genetic algorithms [194],
- auto-catalytic networks [22, 113, 205, 206],
- econophysics [66, 124, 261],
- theory of increasing returns [13],

- origin and statistics of power laws [93, 137, 290, 346],
- mosaic vaccines [31],
- statistical mechanics of complex systems [175, 178, 282, 378],
- networks models in epidemiology [88, 301],
- complexity economics [94, 189, 248, 124],
- systemic risk in financial markets [35, 311],
- allometric scaling in biology [71, 407],
- science of cities [36, 49].

In this book, we want to take a few steps in new directions. In particular, we want to clarify the origin of power laws, especially in the context of driven non-equilibrium systems. We aim to derive a framework for the statistics of driven systems. We try to categorize probabilistic complex systems into equivalence classes that characterize their statistical properties. We present a generalization of statistical mechanics and information theory, so that they finally become applicable and useful for complex systems. In particular, we derive an entropy concept for complex systems and carefully discuss its meaning. Finally, we make an attempt to unify the many classical approaches to evolution and co-evolution into a single mathematical, algorithmic framework. The overarching theme of the book is to contribute to methodology for understanding the co-evolutionary dynamics of states and interactions.