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Complexity Science

The Warwick Master's Course

Edited by
Robin Ball, Vassili Kolokoltsov
and Robert S. MacKay

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Preface

Complexity Science is the study of systems with many interdependent components.

There is an urgent global need from industry, commerce, research institutions, academia, government and public services for a new generation trained to understand how complex systems behave, how to live with them, to control them and to design them well. We see this in public service management, transport, public opinion, epidemics, riots, terrorism, weather and climate. Relevant technological developments include distributed computing, data management, process control, personalised medicine, disease management, environmental sensor swarms, complex materials and nanobiotechnology.

Stimulated by problems from such a wide range of scientific disciplines, it presents great challenges and opportunities for Mathematics. Mathematics is essential for a deep understanding of complex systems and how to quantify their behaviour, for conclusions of genuine value to end-users, because of its powers for description, abstraction, deduction and prediction.

A range of Complexity Science concepts unify the field across disciplines: dynamics and diffusion, interacting agents and networks, coherent structures, emergence and self-organisation, upscaling and model reduction, quantification of complexity, scaling and extreme events, probabilistic modelling and statistical inference, feedback and control, diversity, optimisation and evolution.

This volume presents coherent introductions to the mathematical treatment of some areas of Complexity Science. It is based on some of the lecture modules of the Warwick EPSRC Doctoral Training Centre in Complexity Science.

Chapter 1 by Mario Nicodemi, Yu-Xi Chau, Christopher Oates, Anas

Rana and Leigh Robinson introduces the key themes of Self-Organisation and Emergence. It presents some of the basic examples and tools to illustrate and analyse these phenomena.

Chapter 2 by Yulia Timofeeva treats Complexity in Deterministic Dynamical Systems. Dynamical systems are represented by mathematical models describing phenomena whose instantaneous state changes over time. Examples are mechanics in physics, population dynamics in biology and chemical kinetics in chemistry. One basic goal of the mathematical theory of dynamical systems is to determine or characterise the long-term behaviour of the system using methods for analysing differential equations and iterated mappings. This chapter introduces some of the techniques used in the modern theory of dynamical systems and the concepts of chaos and strange attractors, and illustrates a range of applications to problems in the physical, biological and engineering sciences.

Chapter 3 by Stefan Grosskinsky treats Stochastic Dynamics of Interacting Particle Systems. These are lattice-based stochastic models of complex systems, describing the time evolution of a large number of interacting components or agents, which are simply called particles. The notes provide an introduction to their mathematical description using Markov semigroups and generators, and to basic probabilistic tools for their analysis. The techniques are used to understand collective phenomena and phase transitions as a result of local motion and interaction of the particles for several classes of models. This discussion is mainly example-based. It involves the role of symmetries and conservation laws and provides a connection to concepts from equilibrium statistical mechanics discussed in Chapter 4.

Chapter 4 by Ellák Somfai treats Statistical Mechanics of Complex Systems. This chapter starts by introducing equilibrium statistical mechanics via the maximum entropy principle. This is followed by a phenomenological description of phase transitions and various applications where dynamics plays a critical role, including interface growth and collective biological motion.

Chapter 5 by Colm Connaughton treats Numerical Simulation of Continuous Systems. This chapter provides a foundation in practical methods of obtaining numerical solutions of partial differential equations that arise in complexity science applications. The focus is on understanding the advantages and limitations of numerical methods generally and on selecting and validating an appropriate numerical algorithm when faced with a particular problem. It starts with a basic outline of timestepping methods for ordinary differential equations, then proceeds to cover finite difference methods for hyperbolic and parabolic equations, explicit versus implicit timestepping, issues related to stability, stiffness and singularities, fast Fourier transform and pseudo-spectral methods. It is example-based.

Chapter 6 by Vassili Kolokoltsov is on Stochastic methods in Economics and Finance. It presents theory for utility, risk, optimisation, portfolios, derivatives, fat tails, option pricing and credit risk.

Chapter 7 by Robert MacKay is on Space-Time Phases. The objective is to put the concept of "emergence" onto a firm foundation in the context of dynamics on large networks. The key notion is space-time phases: probability distributions for state as a function of space and time that can arise in systems that have been running for a long time. The chapter has two sections, the first treating the stochastic case of probabilistic cellular automata and the second the deterministic case of coupled map lattices.

Chapter 8, also by Robert MacKay is on Selfish Routing. The chapter is a summary of the very interesting theory of the gap between free market and centrally controlled solutions for many agent systems in an idealised case of traffic flow, following the excellent book by Roughgarden.

We are most grateful to Dayal Strub for typing up the notes of RSM, preparing the figures for RSM and VNK, putting all the files together into the required style and sorting out many issues with typesetting.

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Contents

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Self-organisation and emergence

Mario Nicodemi, Yu-Xi Chau, Christopher Oates,
Anas Rana and Leigh Robinson

Abstract

Many examples exist of systems made of a large number of comparatively simple elementary constituents which exhibit interesting and surprising collective emergent behaviours. They are encountered in a variety of disciplines ranging from physics to biology and, of course, economics and social sciences. We all experience, for instance, the variety of complex behaviours emerging in social groups. In a similar sense, in biology, the whole spectrum of activities of higher organisms results from the interactions of their cells and, at a different scale, the behaviour of cells from the interactions of their genes and molecular components. Those, in turn, are formed, as all the incredible variety of natural systems, from the spontaneous assembling, in large numbers, of just a few kinds of elementary particles (e.g., protons, electrons).

To stress the contrast between the comparative simplicity of constituents and the complexity of their spontaneous collective behaviour, these systems are sometimes referred to as "*complex systems*". They involve a number of interacting elements, often exposed to the effects of chance, so the hypothesis has emerged that their behaviour might be understood, and predicted, in a statistical sense. Such a perspective has been exploited in statistical physics, as much as the later idea of "universality". That is the discovery that general mathematical laws might govern the collective behaviour of seemingly different systems, irrespective of the minute details of their components, as we look at them at different scales, like in Chinese boxes. While the single component must be studied on its own, these discoveries offer the hope that we might understand different classes of complex systems from their simpler examples.

A univocal definition of "complexity" can be elusive, but the above criteria hopefully draw a line to distinguish, in a more technical sense, "complex" from the much broader category of "complicated" systems. Here we introduce some of the basic mathematical tools employed to describe their emergent behaviours. We discuss some basic concepts and several applications (e.g., Brownian motion in physics, asset pricing in finance) of the theory of stochastic processes, which is presented more generally in Chapter 3. We also consider some more advanced topics such as statistical mechanics and its applications to define the emergent properties in interacting systems. The foundations of statistical mechanics are discussed in more detail in Chapter 4. Finally, we introduce more recent topics such as self-organised criticality and network theory.

The course was taught by Mario Nicodemi. The notes that form this chapter were written by Yu-Xi Chau, Christopher Oates, Anas Rana and Leigh Robinson, four students of the Complexity Science Doctoral Training Centre of the University of Warwick who attended the lectures in 2009.

1.1 Random walks

1.1.1 Introduction

Put simply, a **random walk** is a mathematical formalisation of a path a "particle" traces out after taking a sequence of random steps. The idea of a random walk is central to the modelling of a wide range of phenomena, including financial modelling, the diffusion of gases, genetic drift, conformation of polymers, and a large number of other applications where the phenomenon in question evolves by a random process in time.

Various different types of random walk exist but can be grouped into broad categories depending on what the random walker is said to "walk on", and how the time evolution is defined. For example, a random walker may be defined on a graph that evolves in discrete time, moving from one node to another in one discrete time step, or just as well defined would be a random walker that moved in continuous time along the whole real line, $\mathbb{R}$. We shall give no further thought to these kinds of random walks and restrict our discussion to ones that occur along the integers, $\mathbb{Z}$ in discrete time steps.

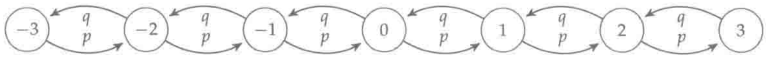

Figure 1.1 A discrete time walk on the integers, $\mathbb{Z}$. Probabilities p and q show how likely that transition is from state to state.

To understand perhaps the simplest example of a random walk we imagine a particle that can inhabit one of the integer points on the number line. At time 0 the particle starts from a specific point and moves in one time step to its next position in the following way: we flip a coin with the result governing how the particle moves. If the coin comes up heads then the particle moves *one* position to the right while if it comes up tails then the particle moves *one* place to the left. If we make n such coin tosses then what will be final position of the particle? Obviously being a random process we can't predict exactly where it will end but we can say a good deal about the distribution of possible outcomes.

1.1.2 One-dimensional discrete random walk

To try and answer such questions we need to introduce some formalism. We define independent random variables, X_i, that can take the values -1 and 1, with $P(X_i = 1) = p$ and $P(X_i = -1) = 1 - p = q$. The X_i represent the direction of the ith step of our random walk. Pictorially we can represent this arrangement as shown in Fig. 1.1. To see how such a system behaves statistically we calculate the first and second moments and variance of X_i as follows:

$$\langle X_i \rangle = \sum kP(X_i = k)_k = 1 \times P(X_i = 1) - 1 \times P(X_i = -1) \quad (1.1)$$

$$= p - (1 - p) = 2p - 1. \quad (1.2)$$

With the second moment and variance given by

$$\langle X_i^2 \rangle = p + (1 - p) = 1, \quad (1.3)$$

$$Var[X_i] = \langle X_i^2 \rangle - (\langle X_i \rangle)^2 = 1 - (2p - 1)^2 \quad (1.4)$$

$$= 1 - 4p^2 + 4p - 1 = 4p(1 - p). \quad (1.5)$$

We now define a new random variable, Z_n, as the sum of n such X_i variables and this defines the distribution of the value of the random walk after n steps:

$$Z_n = \sum_{i=1}^{n} X_i, n > 0. \tag{1.6}$$

We can now look at some of the statistics of Z_n, in particular the average position, $\langle Z_n \rangle$, and the variance: $Var[Z_n]$ of this position:

$$\langle Z_n \rangle = \langle \sum_{i=1}^{n} X_i \rangle = \sum_{i=1}^{n} \langle X_i \rangle = n(2p-1), n > 0. \tag{1.7}$$

Since by definition each of the X_i's are independent the second moment can be easily calculated,

$$\langle Z_n^2 \rangle = \langle (\sum_{i=1}^{n} X_i)^2 \rangle = \sum_{i=1}^{n} \langle X_i^2 \rangle + \sum_{i=1}^{n} \sum_{j=1 i \neq j}^{n} \langle X_i X_j \rangle \tag{1.8}$$

$$= n + n(n-1)(2p-1)^2. \tag{1.9}$$

Hence,

$$Var[Z_n] = \langle Z_n^2 \rangle - (\langle Z_n \rangle)^2 = 4np(1-p). \tag{1.10}$$

In particular, notice that

$$Var[Z_n] \propto n, \tag{1.11}$$

which gives us the result that the variance increases as we walk for more steps. This has important consequences for finance as we shall see later.

Unbiased random walk

So far we have been considering a random walk with general transition probabilities, p and q. The special case where $p = q = 1/2$ is called *unbiased* – since each decision is equiprobable. For these random walks the statistical properties collapse to

$$\langle Z_n \rangle = 0, \tag{1.12}$$

$$Var[Z_n] = \langle Z_n^2 \rangle = n. \tag{1.13}$$

From (1.13) we note that the root-mean-square of Z_n is simply $\sqrt{n}$, which hints that the average absolute distance moved after n steps, $E[\mid Z_n \mid] = O(\sqrt{n})$. This is indeed the case, but will not be proven here. Trajectories for a collection of unbiased random walkers are shown in Fig. 1.2.

A further interesting property of unbiased random walkers is the notion of recurrence. Imagine we choose any point, $i \in \mathbb{Z}$. How many times would you expect the random walker to cross this point if the walker