Stochastic Modelling and Simulation
Introduction

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Data Science and Scientific Computing

COURSE ORGANISATION

LECTURES AND LAB

- “Standard” lectures introducing basic concepts and techniques
- Exercise classes: some exercises, mainly computational

EXAM AND FINAL MARK

- Seminar on a project work: modelling and analysis of a system (to be chosen); implementation project; theoretical seminar.
- Questions on the course topics.
- Exercise sheets can be handled at due dates. Handling successful exercises will give a bonus to the final mark.

TIMETABLE

- 6CFU - 60 hours course (lectures + lab)
- Monday 11-13 and 16-18, and Tuesday 14-18 (not flexible).

Outline

1. Introduction by examples
2. Course topics: an overview
3. Modelling: an introduction

A motivational quote

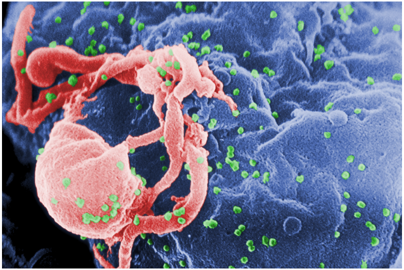
Science is *the* driver of our times.

Stephen Emmott
Microsoft Research, Cambridge, UK

DATA CENTRE EFFICIENCY

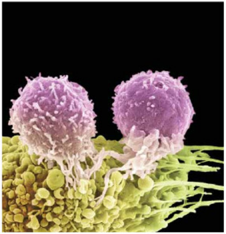
- We want to reply to all customer requests with small latency.
- We want to consume as little energy as possible.
- There is a trade off between these two goals. How many servers do we need to run for a good compromise?

HIV DRUG DOSAGE



- HIV therapies require the assumption of drug cocktails for long periods of time.
- How do we find the best cocktail for a given patient?
- And how do we plan the drug dosage for it to be the most effective for a given patient?

Cancer and the importance of networks

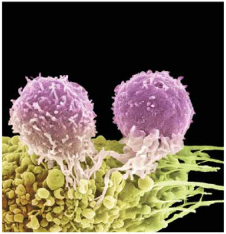


T lymphocytes and cancer cell
Coloured scanning electron micrograph [SEM] of two T lymphocyte cells attached to a cancer

What is cancer?

- Is Cancer a disease of genes?
- Is Cancer a disease of biological pathways?
- Is Cancer a disease of interaction networks?
- Is Cancer a disease of the ecology of cell populations?

CANCER AND THE IMPORTANCE OF NETWORKS



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WHAT IS CANCER?

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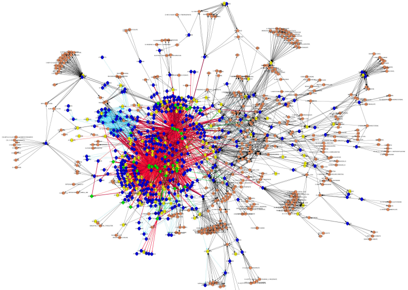
To better fight Cancer, we need to better understand the dynamical aspects of the (gene, protein, cell) interaction networks.

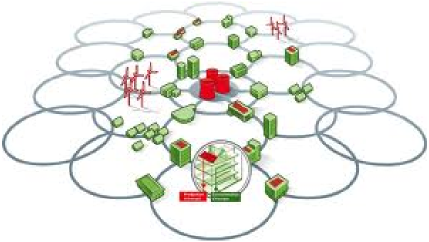
We need large-scale data analysis + modelling



OPTIMAL FISHING POLICY

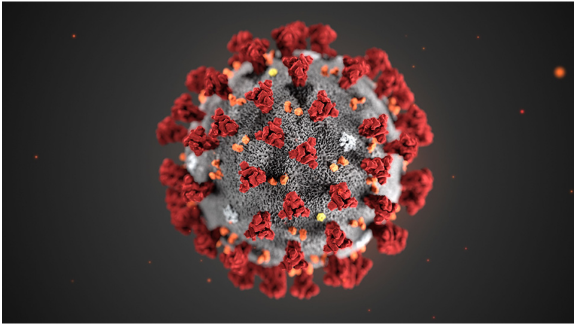
- Fishing alters the equilibrium of the see ecosystem.
- The number of prey and predators tend to follow a cycle at equilibrium (from many preys, few predators to few preys, many predators)
- Can we find a fishing policy that does not destroy the system, but rather stabilises it?

LOAD CONTROL IN SMART GRIDS



- Renewable energies introduce a high volatility and unpredictability in energy production.
- If the demand of energy exceeds the production, then we need to activate standard plants, to to reduce consumption by switching off devices (e.g. water boilers remotely controlled by smart meters).
- What is the optimal policy to achieve this?

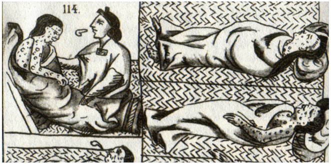
SPREADING OF EPIDEMICS



- Diseases have always had a large influence in human history, and even today their impact can be quite dramatic.
- How can we predict the severity of an epidemic?
- How can we counter-act to a rising epidemic to stop it, e.g. by vaccination or quarantine?

Some (in)famous epidemics

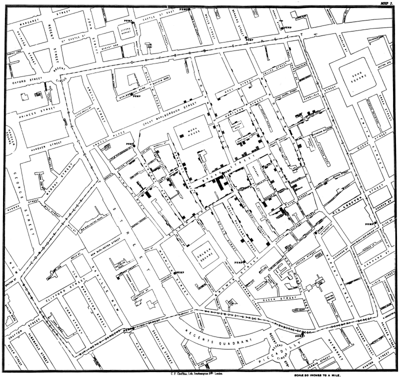
Plague, the Black Death



Smallpox, Mexico, 1500

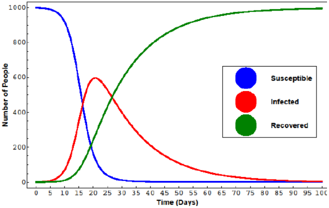
Spanish Flu 1918-19

(MATHEMATICAL) EPIDEMIOLOGY - HISTORY PILLS



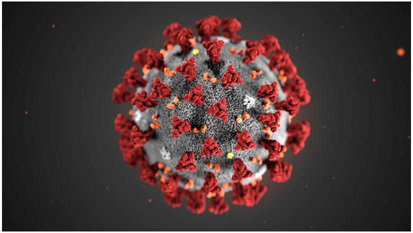
Cholera outbreak, Broad street, London

Kormack and McKendrick



SIR model

How severe will an epidemic be?



This question may be interpreted in a variety of ways. For example, how many individuals will be affected altogether and thus require treatment? What is the maximum number of people needing care at any particular time? How long will the epidemic last? How much good would quarantine or isolation of victims do in reducing the severity of the epidemic?
These are some of the questions we would like to study with the aid of models.

Brauer, Mathematical Epidemiology, 2009

Epidemic Modelling

Epidemic Modelling

Table 2.1 Eyam Plague data

Date (1666)	Susceptibles	Infectives
July 3/4	235	14.5
July 19	201	22
August 3/4	153.5	29
August 19	121	21
September 3/4	108	8
September 19	97	8
October 4/5	Unknown	Unknown
October 20	83	0

The relation (2.3) with $S_0 = 254$, $I_0 = 7$, $S_\infty = 83$ gives $\beta/\alpha = 6.54 \times 10^{-3}$, $\alpha/\beta = 153$. The infective period was 11 days, or 0.3667 month, so that $\alpha = 2.73$. Then $\beta = 0.0178$. The relation (2.4) gives an estimate of 30.4 for the maximum number of infectives. We use the values obtained here for the

COURSE TITLE EXPLAINED

- All the scenarios presented are examples of complex systems.
- When we model these systems, we need to consider our uncertainty about them in a consistent way.
- Stochastic modelling provides effective and mathematically grounded tools in this direction.
- These models are typically impossible to solve analytically: we need efficient computer simulation.

Outline

AN HIGH LEVEL VIEW ON CS

HIGH LEVEL VIEW

We will look at complex systems as systems made up of entities interacting in complex ways.

ENTITIES?

Entities can be of different nature: molecules, cells, animals, computer jobs, processors, humans, ...

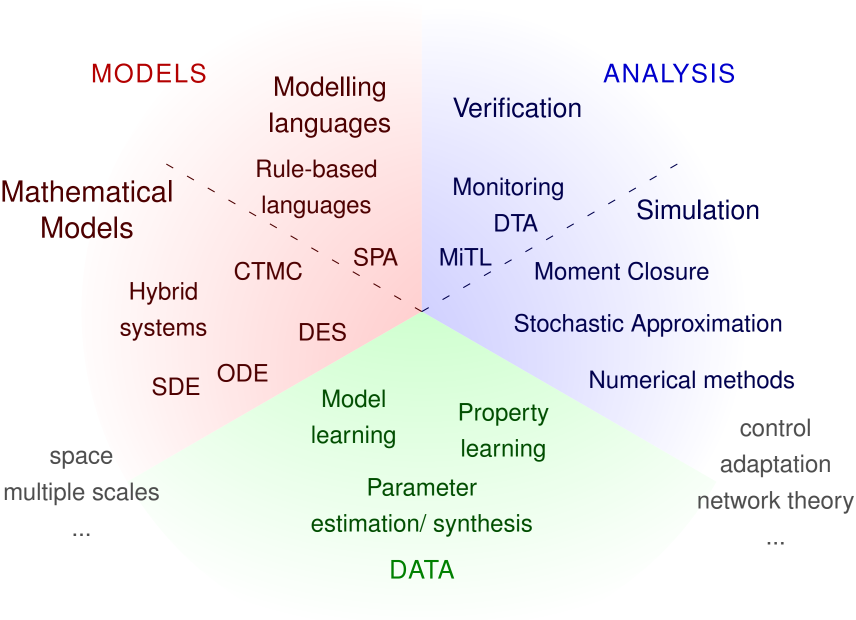
INTERACTIONS?

Interactions can involve a small or large number of entities, and may depend in complex ways from the environment or the global state of the system (non-linearity)

FEATURES

Non-linearity, emergent behaviour, self-organization, adaptivity, openness, robustness, evolutionary aspects, ...

A MAP OF COURSE TOPICS



COURSE TOPICS

- Foundations of probability and
- Simulation of random variates (sampling)
- Discrete Time Markov Chains
- Markov Chain Monte Carlo
- Discrete Event Simulation and statistical analysis
- Continuous Time Markov Chain
- Population models and applications
- Simulation of population models
- Approximation of population models (i.e. mean field)
- Parameter inference from data

POSSIBLE CASE STUDIES

- Systems/synthetic biology: gene networks, signalling networks, ...
- Epidemiology: epidemic spreading, network epidemics, ...
- Computer systems: queueing networks, ...
- (?) Ecology: prey-predator dynamics, ant foraging, ...
- (?) Crowd modelling: “el bottellón”, emergency egress, ...
- (?) Smart cities: smart grids, bus networks, bike sharing
- ...

Course topics: word of warning

1. The previous list is by no means exhaustive.
2. If you want to discuss something different (a different theoretical approach, other case studies), feel free to ask and negotiate.
3. We will not cover the material in full detail. I would rather like to introduce you to the main ideas, so you can explore the topics you like more (if any).

Outline

A motivational glance

Science is *the* driver of our times.

Stephen Emmott
Chief of Computational Sciences
Microsoft Research Cambridge

Human society faces many challenges...

What do climate, crops growth, economy, societies, epidemic outspread, life beings, tumors, cells, and so on, have in common?

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What do climate, crops growth, economy, societies, epidemic outspread, life beings, tumors, cells, and so on, have in common?

They are all complex systems

HUMAN SOCIETY FACES MANY CHALLENGES...

What do climate, crops growth, economy, societies, epidemic outspread, life beings, tumors, cells, and so on, have in common?

They are all complex systems

Facing these challenges passes through our ability to understand their functioning and control their behaviour.

Human society faces many challenges...

What do climate, crops growth, economy, societies, epidemic outspread, life beings, tumors, cells, and so on, have in common?

They are all complex systems

Facing these challenges passes through our ability to understand their functioning and control their behaviour.

This is *the* major scientific challenge of the 21^{st} Century!

A motivational glance

Computational Science is *the* driver of our times.

Paraphrasing Stephen Emmott :-)

A motivational glance

Computational Science is *the* driver of our times.

Paraphrasing Stephen Emmott :-)

The level of complexity, the size of those systems, the large amount of experimental data, require vast computational power to be processes.

And clever mathematics and algorithms to do it!!
Beyond the current state of the art...

What is a complex system?

from Wikipedia

A complex system is a system composed of interconnected parts that as a whole exhibit one or more properties (behavior among the possible properties) not obvious from the properties of the individual parts.

The original Latin word complexus signifies entwined or twisted together (Heylighen, 1996).

Examples of complex systems

Complex systems are ubiquitous in the world.

- Biological systems
- Ecological systems
- Physical systems
- Computer systems
- Socio-economical systems
- ...

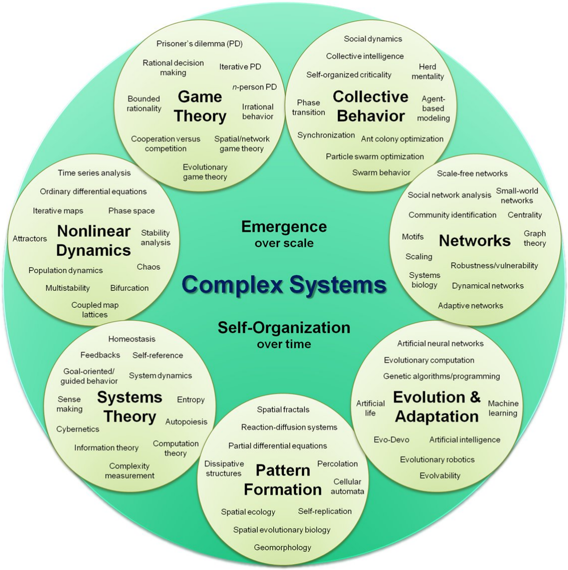
COMPLEXITY

Complexity can be defined as “the name given to the emerging field of research that explores systems in which a great many independent agents are interacting with each other in many ways” [Waldrop, 1992]

Complexity is characterised by non-linear relationships between parts, openness, feedback loops, emergence, pattern formation, and self-organisation (Grobbelaar and Ulieru, 2007).

from R. Frei, G. Di Marzo Serugendo: Concepts in complexity engineering. IJBIC 3(2): 123-139 (2011).

FEATURES OF A COMPLEX SYSTEM



Emergent Behaviours

Emergence describes how order appears out of chaos.
Holland, 1998

Emergence results in a self-organised increase of order, in space or time. A global behaviour arises from the interactions of its local parts; cannot be traced back to the individual parts (De Wolf and Holvoet, 2005).

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An example: El Bottellón.

El bottellòn refers to a phenomenon in the city of Granada, Spain: people in the nights spontaneously gather in a square in the city and start a big drinking party.

Adaptivity and self-organization

"Self-organisation is the dynamical and adaptive mechanism or process enabling a system to acquire, maintain and change its organisation without explicit external command during its execution time; there is no centralised or hierarchical control. It is essentially a spontaneous, dynamical (re-) organisation of the system structure or composition."

Adaptation means achieving a fit between system and environment; thus, every self-organising system adapts to its environment (Heylighen, 2003).

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Adaptivity and self-organization

Self-organization is strongly related to the concept of emergence.
It usually refers to systems that are made up of atomic components that have a form of “intelligence” (i.e. small robots, bird flocks, schools of fishes).

An high level view on CS

High level view

We will look at complex systems made up of entities interacting in complex ways (population models).

Entities?

Entities can be of different nature: molecules, cells, animals, computer jobs, processors, humans, ...

Interactions?

Interactions can involve a small or large number of entities, and may depend in complex ways from the environment or the global state of the system (non-linearity)

Features

Non-linearity, emergent behaviour, self-organization, adaptivity, openness, robustness, evolutionary aspects, ...

Modelling complex systems

Essentially, all models are wrong, but some are useful.
George E. P. Box

What is modelling?

Modelling means constructing a formal object, based on some mathematics, which is an abstract representation of the reality. As such, any model is wrong. But we hope it to be sufficient to *capture some aspects of the phenomenon studied*.
Any model of complex systems requires experimental data to be tuned and validated.

Modelling complex systems

The goals of modelling

Modelling has two main goals: explanation and prediction.

Explanation: identify the key ingredients that drive the observed behaviour of the phenomenon of interest.

Prediction: predict the behaviour of the system under different situations.

These two goals are somehow in conflict for complex systems: explanation calls for abstraction, prediction for detail.

Qualitative versus quantitative

Models can be qualitative, essentially capturing possible behaviours, but without giving “numbers”, or quantitative, giving quantitative predictions of measurable quantities (when and if measurement is possible).

Modelling complex systems

Maths for quantitative models

We will be interested in the temporal behaviour of systems.
We will consider some key ingredients for the maths:

Entities: can be modelled as discrete objects or continuous quantities.

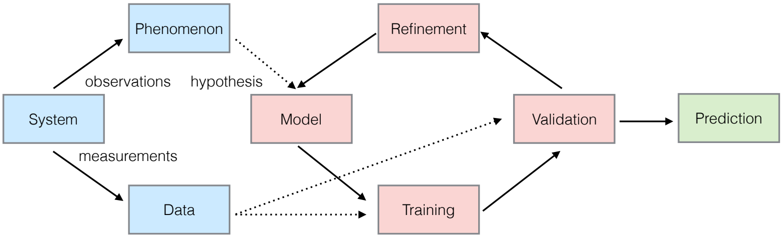
Evolution: can be (non)-deterministic or stochastic.

Time: can be discrete or continuous.

By choosing a combination of the ingredients above, we obtain different mathematical objects to work with:

- Discrete or continuous time Dynamical systems (DTDS, ODE, PDE, SDE);
- Stochastic Processes (discrete or continuous time Markov Chains)
- Hybrid systems (a mixture of the above)

Modelling cycle



Important issues

Validation Model has to be fitted to experimental data and then validated in its explicative/predictive power.

Data problem Technological improvements permit the generation of huge amount of data. One needs to make sense of them.

Computational problem Model simulation and analysis can be extremely costly from a computational viewpoint (large models), but also model fitting and data analysis.

Data-based vs Model-based Approaches

Will data-based approaches make this kind of modelling obsolete?

- Data-based methods are still model-based, yet models like deep neural networks are very powerful but black-box. Explanatory power is missing (cf. Explainable AI). Plus they do not make use of available knowledge.
- Mechanistic models have much more explanatory power, and are based on existing knowledge. But it can be hard to build a good model - this requires a lot of expertise.
- The most likely outcome is an hybrid approach that bridges these two worlds...