Intro to the Topic
Discrete Models
Growth and Decay
Linear & Non-Linear Interaction Models

CA659
Mathematical Methods/
Computational Science

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Chapter 1:

Introduction & Basics

Recommended Books for the Course

Intro to the Topic
Discrete Models
Growth and Decay
Linear & Non-Linear Interaction Models

Assessment

- Exam in May
- Three hours
- Attempt Any Four from Six Questions

Tutorials

- Tutorial/Workshop every week
- One hour long?
- Some questions from tutorials will feature on the exam

What is Data Analytics?

A Gartner\(^1\) Definition:

'Analytics has emerged as a catch-all term for a variety of different business intelligence (BI)- and application-related initiatives . . . Increasingly, “analytics” is used to describe statistical and mathematical data analysis that clusters, segments, scores and predicts what scenarios are most likely to happen. 'Whatever the use cases, “analytics” has moved deeper into the business vernacular. Analytics has garnered a burgeoning interest from business and IT professionals looking to exploit huge mounds of internally generated and externally available data.'

\(^1\)i.e. business-oriented
What is a Model?

A model is an abstraction or representation of something and can be either:

- An *iconic model* (e.g. airplane in a wind tunnel) represents the system with assumptions, giving a simplified picture of what is actually happening and resembles the real thing with observable effects.

- A *mathematical model* (e.g. models of planet undergoing climate change) is a symbolic model of some physical (i.e. climate) or conceptual (e.g. a budget) subject matter including concepts not visually apparent. It is a math model describing a system using math concepts and language. For some problems, the mathematics are not tractable and we must use Probabilistic/Stochastic techniques.

Characteristics of a Model

- It highlights features of interest without manifesting the ‘unnecessary’ detail.

- It is cheaper, more convenient, and safer to manipulate than the real-world equivalent.

- It is deterministic in that it produces (with the same input) the same results every time you run it, unlike experiment.
Dissolution of a tablet in the digestive system

In this case the model takes what is an inherently complex (multiple dissolution environments and idiosyncrasies of individuals), experimentally expensive (difficult, expensive and non-deterministic) and ethically controversial (with human/animal experiments) system and replaces it with one which is Cheap, deterministic and can model however many layers of detail are desired.


**Figure 1.1:** Drug Dissolution In-Vitro Modelling
Modelling of Option Pricing in Financial Systems

Here what is sought is a predictive model for the effects on the price of a particular financial derivative instrument as a function of time. Given the Black-Scholes Formula can calculate the price of an option as a function of time.

Computational science is the application of computational and numerical techniques to solve large and complex problems. It takes advantage of not only the improvements in computer hardware, but more importantly, the improvements in computer algorithms and mathematical techniques.

Computational Science is the intersection of three disciplines:

Figure 1.4: A Schematic of Computational Science

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2Shodor Education Prog shodor.org/chemviz/overview/compsci.html
In Fig. 1.5, computational science is a branch of science (application) that is supported by the mathematical methods (algorithms) and computer science (architecture). Computation now is widely accepted, along with theory and experiment, as a crucial third mode of scientific research and engineering design.

**Figure 1.5**: Another View of Computational Science

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In the application of computational science to real-world problems it is necessary to decide the following:

- What scientific event or problem is the focus of our interest?
- What are its boundaries and what is external to the system in question?
- What are the system’s component parts and how much detail should we include?
- What assumptions can be made about its behavior?
- Have other systems been studied similar to the one in question?

Once these key decisions have been made, then we can put together the necessary mathematical model to represent the behaviour of the problem.
What is a Data Analyst/Data Modeller?

As a Data Analyst/Modeller, you would be looking at the following properties of the data:

- Where does it come from? Human/Machine, Single/Multiple Sources?
- Has it been altered/filtered already?
- Is there a lot of it (i.e. for model training/evaluation)?
- What is the granularity?
- How clean is it/Is it noisy?
- What are the units?
- What are its properties?

Remember: Data is someone’s IP and is treated as such by them!

Data Analytics & Developments in Computing

As noted above, developments in Computing (Computer Architecture & Computer Science) have contributed to a resurgence in Computational Science.

In particular, we note developments such as:

- Decrease in memory costs with consequent increase in storage capabilities (e.g. Amazon S3)
- Increase in processing power allied to decreases in costs (From $10^{8}$USD/FLOP to $10^{-8}$USD/FLOP!)
- Increases in Internet network speeds up to $10^{10}$ bits per s
- Data availability from multiple sources (smartphones and other pervasive computing sources)

These may be seen as key enablers in Data Analytics.
Alongside DA, have ‘Big Data’ and it’s cousin ‘Big Services’.

- Industry is full of a lot of hype surrounding ‘Big Data’
- But increasing with it is Big Data’s cousin Big Services.
- Started as design guidelines for the creation of reusable services, and evolved to Service-Oriented-Architecture (SOA)
- When Software-as-a-Service (SaaS) is added, SOA’s contribution to B2B talk becomes considerable
What has DA, have as ‘Big Data’. Some facts:\(^3\)

\textbf{Volume}
- Up to 2003, we created \(5 \times 10^{16}\) Bytes of Data.
- In 2011, generated the same every two days.
- In 2013, same created every 10 minutes.
- In Future???

\textbf{Variety}
- Different types of data structured and unstructured data (e.g. text, sensor data, audio, video, -omics ...).
- Estimated 2 billion smartphones on planet in 2015 churning out sensor data.
- Defence/Government monitor live video feeds from \(5 \times 10^{8}\) of surveillance cameras.

Add the other \(V\)’s: \textbf{Velocity} \& \textbf{Veracity}...

\(^3\)Source IBM

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How do these topics fit in together?

\textbf{Figure 1.6} : Big Data Analytics (horicky.blogspot.ie)

In CA659, we will be looking at some parts in \textbf{Orange and Green}.

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Sensor Data Analysis

- Data from sensors on wearer’s body (or from smartphone)
- Wearers can be Seniors or Athletes (or ...)
- For Seniors often the use-case is memory-related (use to refresh memory of events)
- For Athletes, purpose is often performance-related.

Figure 1.7: Image Data From Sensors

Sensor Data Analysis (cont’d) The Data

- Usually long-run time series (image or sensor data)
- Often quite noisy with gaps
- This is due to the reliability of the sensors & network

The Research Questions

- Is there periodicity present in the data?
- If so, does Granularity Analysis reveal anything?
  - are there ‘events’ across time scales?
  - what of memory interest could they highlight?
  - are events correlated among sensors (i.e. IR, picture, accelerometer)?

For athletes’ sensor data, can ask the questions:

- is the performance of the team as a whole optimal?
- is any individual an outlier in under-performance?
Betting Data Analysis

- Betting data from websites from betting ‘agents’
- Each ‘agent’ has own strategy (loyalty, motivation) & profile
- Both of these are of interest to betting companies
- Of equal (or maybe greater?) interest is what they as a whole can say.

The Data

- Again multiple long-run time series (odds data)
- One time series for each outcome
- Market varies from very liquid (major tennis) to illiquid (low league)
- Good quality, non-noisy data in the main
- Web companies don’t like releasing data (IP!)

Examples of Deep Analytics (cont’d)

Betting Data Analysis (cont’d) Research Questions

- Are there ‘outlier’ matches (“home underdogs”/“longshots”), not accurately priced by bookmakers?
- What are the most valuable customers?
  - who places the highest bets?
  - who takes the most risks?
  - do they need to be tracked (insider information, minimize losses)?
- What are the major movements in the data (real-time)?
- Can this be used to optimize ‘cashout’?
- What is the likely effect on outcomes if sudden (unexpected) events happen?
  - unexpected sending off or penalty?
  - key player injured?
Origins of the Module

- This course started off in life as a Computational Biology module.
- It still retains much of that sort of flavour.
- The reason for this is that many of the problems examined involve time-dependent situations.
- Also many of the models that we use build on those developed in earlier times.
- An example would be Rumour Spread using a model for Infectious Diseases.

Maths Content in the Module

Many of those taking this and previous versions of the module have asked whether a knowledge of Higher Level Maths was a prerequisite for the module.

- We will cover much of the necessary supplementary material in the course.
- There will be topics that you would be expected to familiarise yourself with:
  - Basic probability
  - Basic matrix operations
  - Graph plotting
  - Calculus
- There will be tutorials and worked examples in the course.
In the CA659 Module we will cover modelling topics such as:

- Modelling with Linear & Non-linear Difference Equations
- Continuous Models of Growth & Decay
- Linear & Non-linear Models of Interaction

If time permits, we will look at topics such as:

- Time series analysis
- Examples of research problems.