

# CA659 Mathematical Methods/ Computational Science

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## Assessment

### Assessment

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

### Tutorials

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

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## What is Data Analytics?

A Gartner<sup>1</sup> Definition:

‘Analytics has emerged as a catch-all term for a variety of different business intelligence (BI)- & application-related initiatives . . . Increasingly, “analytics” describes **statistical** and **mathematical data analysis** that clusters, segments, scores and predicts what scenarios are most likely to happen.

‘Whatever the use cases, “analytics” has become a hot business topic, gathering interest from business and IT professionals like looking to exploit huge mounds of internally generated & externally available data.’

<sup>1</sup>i.e. business-oriented

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## Mathematical Modelling: What is a Model?

A model is an abstraction or representation of something.  
Could be:

- An *iconic model* (e.g. airplane in a wind tunnel)
  - represents the system with assumptions,
  - gives a simplified picture of what actually happens
  - resembles the real thing with observable effects.
- A *mathematical model* (e.g. models of planet undergoing climate change)
  - symbolises some physical (i.e. climate)/ conceptual (e.g. budget) subject
  - includes concepts not visually apparent
  - math models the system with math concepts & language.

For some problems, maths are not tractable - must use Probabilistic/Stochastic techniques.

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## Mathematical Modelling: What is a Model? (cont'd)

Characteristics of a Model

- highlights features of interest without manifesting the 'unnecessary' detail.
- is cheaper, more convenient, and safer to manipulate than the real-world equivalent.
- is deterministic i.e. produces (on same input) same results on running it, unlike experiment.

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## Mathematical Modelling: Example 0.1

- *Tablet Dissolution in a digestive system: system features*
  - physically complex (multiple dissolution environments & individual differences)
  - also experimentally expensive (difficult, expensive & non-deterministic)
  - ethically controversial (with human/animal experiments)

*Model features:* cheap, deterministic & can include lots of detail

*Maths required:* Differential equations (advection & diffusion)

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## Mathematical Modelling: Example 0.1 (cont'd)

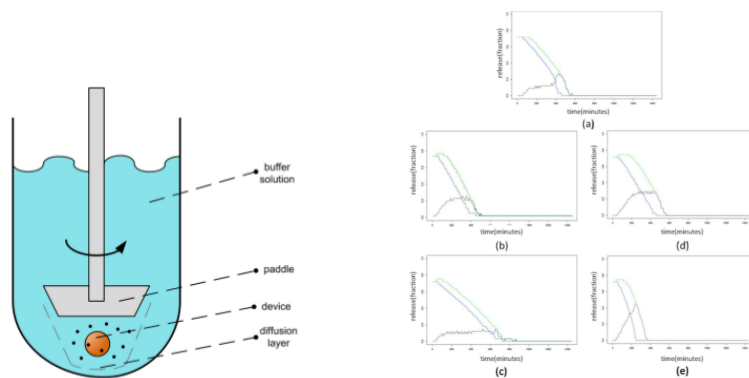


FIGURE 1.1 : Drug Dissolution In-Vitro Modelling

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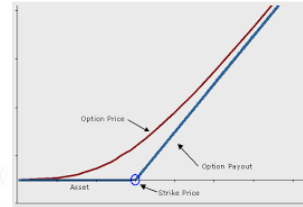
## Mathematical Modelling: Example 0.2

- *Modelling of Option Pricing in Financial Systems*
  - need price of a particular financial instrument with time.
  - must solve the *Black-Scholes Formula*

*Maths required:* Stochastic Partial Differential Equations.

$$\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0$$

(a) Black-Scholes Eqn



(b) Option Price Plot

FIGURE 1.2 : Option Pricing

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## Computational Science: What is it?

‘the application of computational & numerical techniques to solve large and complex problems. [It] takes advantage of not only improvements in [computer hardware](#), but more importantly, the improvements in [algorithms](#) & [mathematical techniques](#).’<sup>2</sup>

Computational Science is the intersection of three disciplines:

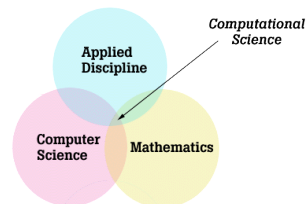


FIGURE 1.3 : A Schematic of Computational Science shodor.org

<sup>2</sup>Shodor Education Prog

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## Computational Science: What is it(cont'd)

In Fig. 1.4,

- computational science is a branch of science (application)
- supported by the mathematical methods (algorithms)
- and computer science (architecture).

Along with theory and experiment, it's crucial third mode of scientific research & design.

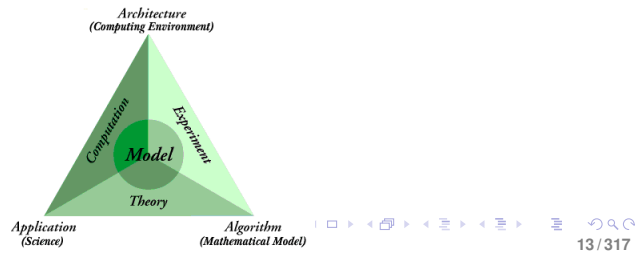


FIGURE 1.4 : Another View of Computational Science shodor.org

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## Computational Science: What is it?(cont'd)

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

- 1 What scientific event or problem is in focus?
- 2 What are its boundaries & what is external to the system?
- 3 What are the system's parts & what detail should we include?
- 4 Any assumptions to be made about its behavior?
- 5 Have other systems been studied akin to this one?

Once these key decisions have been made, then we can put together the necessary mathematical model to represent the behaviour of the problem.

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## What is a Data Analyst/Data Modeller?

As Data Analyst/Modeller, you look at following data properties:

- Origins? 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?

NB: Data is someone's IP and is treated as such by them!

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## Data Analytics & Developments in Computing

Computing advances (esp. memory costs & processor speed) have driven Computational Science.

In particular, we note developments such as:

- 1 Memory costs decrease with increase in storage capabilities (e.g. Amazon S3)
- 2 Processing power rise with reduced cost (From  $10^8$ USD/FLOP to  $10^{-8}$ USD/FLOP!)
- 3 Increases in Internet network speeds up to  $10^{10}$  bits per s
- 4 Data availability from multiple sources (smartphones & sensors)

These may be seen as key enablers in Data Analytics.

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## Data Analytics & Big Data

Data Analytics 'chews on' 'Big Data'. Some facts:<sup>3</sup>

1 *Volume*

- Up to 2003, we created  $5 \times 10^{18}$  Bytes of Data.
- In 2011, generated the same every two days.
- In 2013, same created every 10 minutes.
- In Future???

2 *Variety*

- Types un/structured data (e.g. text, audio, video, -omics).
- Est.d 2 Bn smartphones in 2015 giving out sensor data.
- Govt monitors live video feeds from  $5 \times 10^8$  of surveillance cameras.

Add the other V's: *Velocity* & *Veracity*...

<sup>3</sup>Source IBM

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## Data Analytics & Big Data (cont'd)

How do these topics fit in together?

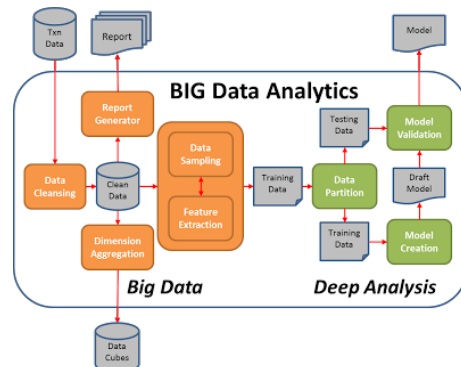


FIGURE 1.5 : Big Data Analytics (horicky.blogspot.ie)

In CA659, we examine some parts in Orange and Green.

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## Examples of Deep Analytics

### 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.

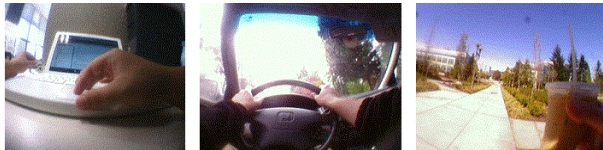


FIGURE 1.6 : Image Data From Sensors

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## Examples of Deep Analytics (cont'd)

### Sensor Data Analysis (cont'd)

#### The Data

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

#### 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?

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## Examples of Deep Analytics (cont'd)

### *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!)

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## Examples of Deep Analytics (cont'd)

### *Betting Data Analysis (cont'd)* Research Questions for Company

- What are the most valuable customers? (places big bets? takes 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 happens to outcomes with unexpected events (e.g. sending off/ penalty)?

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## Origins of the Module

- 1 Course began life as a Computational Biology module.
- 2 It still retains much of that sort of flavour.
- 3 Many problems examined involve time-dependent situations.
- 4 For this reason time series are covered in some depth.
- 5 Many models build on those developed in earlier times.
- 6 An example would be Rumour Spread using a model for Infectious Diseases.

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## Maths Content in the Module

Is a knowledge of Higher Level Maths a prerequisite?/

- 1 We cover many supplementary topics in the course.
- 2 There will be topics that you are expected to be familiar with:
  - Basic probability
  - Basic matrix operations
  - Graph plotting
  - Calculus
- 3 There will be tutorials many weeks in the course.

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## Topics Covered in CA659

In the CA659 Module we will cover modelling topics such as:

- 1 Time series analysis
- 2 Modelling with Linear & Non-linear Difference Equations
- 3 Continuous Models of Growth & Decay
- 4 Linear & Non-linear Models of Interaction

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Chapter 1:

## Time Series Modelling

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