MATH 3290 Mathematical Modeling

Overview of the course

Kuang HUANG

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Department of Mathematics
The Chinese University of Hong Kong

People

Instructor

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Class time and venue

Lecture

- Wednesday 9:30AM - 10:15AM, Science Centre L5;
- Friday 9:30AM - 11:15AM (15-min break), Mong Man Wai Bldg 710.

Tutorial

- Wednesday 8:30AM - 9:15AM, Science Centre L5.
- NO tutorial this week.

Course Webpage

https://www.math.cuhk.edu.hk/course/2324/math3290

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Course description

This course is an introduction to mathematical modeling.

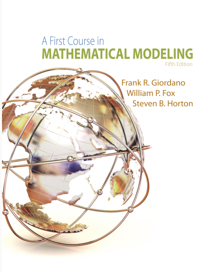
We will cover some basic mathematical tools for the quantitative description of practical problems arising from physics, biology, economics and engineering. The use of these mathematical models allows us to quantitatively study and provide solutions to these problems.

The focus of this course is to give an overview of the mathematical techniques that are commonly used in practice, and illustrate the modeling procedure through some elementary examples.

You will get a taste of mathematical modeling.

Textbook

We will follow closely:



A First Course in Mathematical Modeling by Giordano, Fox, Horton and Weir (5th Edition).

Lecture slides will be released at the course webpage. We will not provide hard copies.

Outline of the course

- The Modeling Process
- Modeling Change
- Model Fitting
- Experimental Modeling
- Simulation Modeling
- Optimization of Discrete Models
- Optimization of Continuous Models
- Modeling Using Graph Theory
- Modeling with a Differential Equation
- Modeling with Systems of Differential Equations

Your background

You should be good at

- Linear algebra (e.g. MATH 1030, 2040);
- Multivariable calculus (e.g. MATH 2010, 2020);
- Computing (e.g. MATLAB, Python, C, C++, Excel, $\cdots$).

Remark: The models we will discuss are deterministic models. We will skip the discussion on most stochastic models, as these require knowledge in probability theory which is not assumed in this course, while stochastic models are widely used too.

Assessment scheme

Your final grade depends on the following.

- **Assignment** (15%)
  - 3-4 assignments in total.
  - Both theoretical and computational (MATLAB, Python, Excel or C).
  - 1 – 2 problems will be graded for each assignment due to limited manpower.
  - You are encouraged to work on optional problems.
  - Submitting your assignments via Blackboard, late submissions are not allowed.
- **Midterm** (35%), March 15, a closed-book 90-min exam.
- **Final** (50%), TBA, a closed-book two-hour exam.

Code of academic honesty

- Very high importance on honesty in academic work submitted by students.
- Zero tolerance on cheating and plagiarism.
- Any related offense will lead to disciplinary action including termination of studies.

Honesty in Academic Work: A Guide for Students and Teachers

Don't Panic

- "All models are wrong, but some are useful"
  - This is not a pure mathematical course, we will seldom talk about theorems, lemmas etc.
  - Simple models are not always useful, but popular.
- "Rome wasn't built in a day"
  - In most scientific disciplines, mathematical models are ubiquitous.
  - The legacy from my own "Mathematical Modeling" course is the coding ability.
  - You may participate in some mathematical modeling contests (MCM/ICM and CUMCM).

Some suggestions about computing languages/tools

Some assignments need you to write codes. However, computing performance/efficiency is not in our consideration, while the primary goal is implementing algorithms and outputting your results in graphs or tables.

Matlab

(Pros)

- Out-of-the-box usage
- A lot of built-in functions
- Easy to draw graphs
- Free student license...

(Cons)

- Expensive out of the school
- Limited usages beyond academic areas
- Personally, indexes in Matlab start from 1...

Some suggestions about computing languages/tools

Python (Anaconda)

(Pros)

- Popularity, the default choice in machine learning...
- Anaconda (NumPy + SciPy + Matplotlib) provides all you needed
- Totally free and open
- It is a general programming language...

(Cons)

- Computing performance may not be satisfying (still at the same level with Matlab)

Some suggestions about computing languages/tools

Excel

(Pros)
- user-friendly
- Easy to perform data analysis (draw figures)...

(Cons)
- Programming on it may not be straightforward (Excel VBA)...

C/C++, Fortran

(Pros)
- Extremely efficient!

(Cons)
- Extremely hard to configure for beginners
- It will be too heavy to perform data visualizations...

Announcements

- Jan 17: a review of Python and MATLAB during tutorial time.
- The slides can be downloaded from the course webpage.
- The assignments should be submitted to Blackboard.
- Please check both the course webpage and Blackboard regularly.
- Midterm: Mar 15, a closed-book 90-min exam.

Timetable

Week	Tut.	Lec.	Lec.	
1	1-10	1-10	1-12	Chap. 0, 2
2	1-17	1-17	1-19	Chap. 1
3	1-24	1-24	1-26	Chap. 3, 4
4	1-31	1-31	2-2	Chap. 4
5	2-7	2-7	2-9	Chap. 4, 5
6	2-14	2-14	2-16	Chap. 5
7	2-21	2-21	2-23	Chap. 5, 7
8	2-28	2-28	3-1	Chap. 7, 13
9	3-6	3-6	3-8	
10	3-13	3-13	3-15	
11	3-20	3-20	3-22	Chap. 8
12	3-27	3-27	3-29	Chap. 8, 11
13	4-3	4-3	4-5	Chap. 11
14	4-10	4-10	4-12	Chap. 12
15	4-17	4-17	4-19	Chap. 12

=No classes

=Review class

=Midterm

Brief description of contents

Topics:

- Modeling by difference equations
- Model fitting and empirical modeling
- Mathematical tools for big data analysis
- Simulation modeling
- Modeling by graph theory
- Optimization modeling, both discrete and continuous
- Modeling by differential equations

Modeling by difference equations

Use difference equations to describe some behaviors, such as

$$a_{n+1} = 3a_n + 2, \quad b_{n+1} = 2b_n + 5b_{n-1}.$$

In above, a_n, b_n represent quantities of interest, and n usually represents time. These are relations of quantities of interest at various times.

One can use this to model (for example):

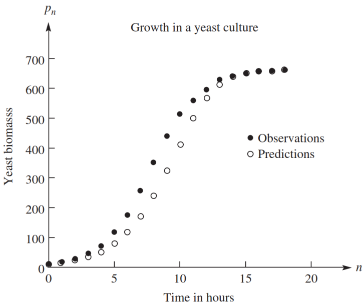
- some financial quantities, such as, loan, interest, ...
- drug concentration for medical applications,
- voting behaviors,
- ...

For example, we obtain the following model based on observations:

$$p_{n+1} = p_n + 0.00082(655 - p_n)p_n,$$

where p_n is concentration of yeast at time n.

Time in hours	Observation	Prediction
0	9.6	9.6
1	18.3	14.8
2	29.0	22.6
3	47.2	34.5
4	71.1	52.4
5	119.1	78.7
6	174.6	116.6
7	257.3	169.0
8	350.7	237.8
9	441.0	321.1
10	513.3	411.6
11	559.7	497.1
12	594.8	565.6
13	629.4	611.7
14	640.8	638.4
15	651.1	652.3
16	655.9	659.1
17	659.6	662.3
18	661.8	663.8



One can use this model for predictions.

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Model fitting

To find a mathematical relationship among variables.

Typically, some known mathematical formulas are assumed, and one needs to determine unknown parameters (also called parameter identifications).

For example, the variable y depends on the quantities x and w. It is known that the relation has an expression

$$y = af(x) + bg(w) + ch(x, w),$$

where $f(x)$, $g(w)$ and $h(x, w)$ are given functions.

We then use some mathematical principles to find the parameters a, b and c that best describe the data.

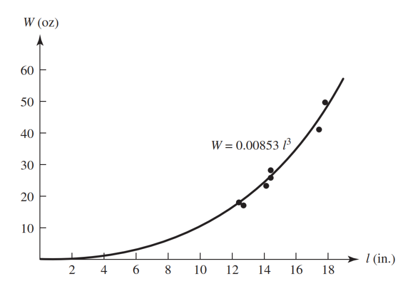
Assume you are interested in finding the relationship between weights W and lengths l of a certain kind of fish, and the following observations are obtained.

Length, l (in.)	14.5	12.5	17.25	14.5	12.625	17.75	14.125	12.625
Weight, W (oz)	27	17	41	26	17	49	23	16

Note, the weight (precisely, mass) should be a function of the volume.
Therefore, one should fit

$$W = c\, l^3,$$

where c is a parameter.



Empirical modeling

To find a mathematical relationship among variables.

The exact mathematical relations among the variables are not known.

For example, the variable y depends on the quantities x and w. We need to find $f(x, w)$ such that

$$y = f(x, w).$$

This problem is harder. Typically, one needs to get some measurement data.

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Big data analysis

Given a set of n data points $x_j \in R^d$. We typically assume both n and d are large.

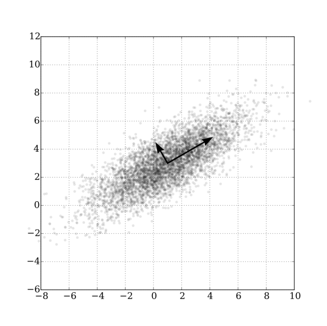
There are two important questions:

- how to get the main feature of the data, and perform data compression,
- how to divide the data into groups, i.e., data clustering.

Getting main features of data points

How to obtain main features?

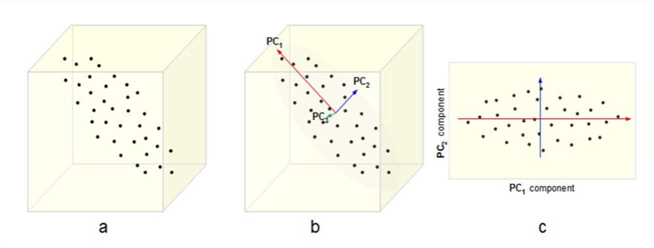
How to extract main "directions" in a given data set?



In high dimensions, this is not easy, while principal component analysis (PCA) is a good tool.

Application

One can perform dimensional reduction (data compression).

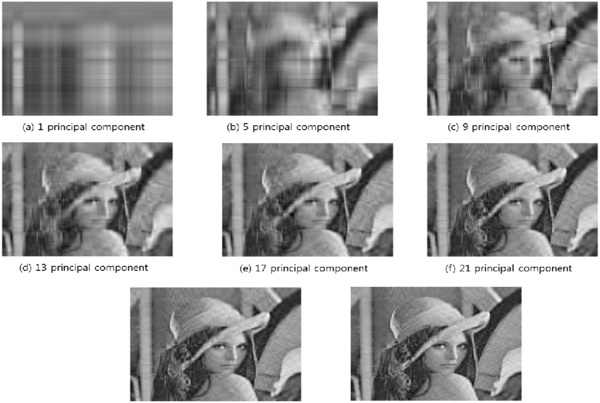


a: A given data set in high dimension.

b: There are two main directions, called PC_1 and PC_2.

c: One can project the data into a 2D (=two-dimensional) space.

Using different numbers of principal directions:



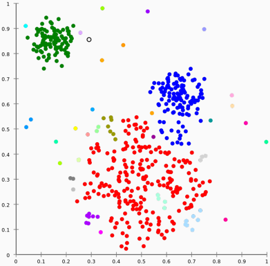
(a) 1 principal component
(b) 5 principal component
(c) 9 principal component
(d) 13 principal component
(e) 17 principal component
(f) 21 principal component
(g) 25 principal component
(h) 29 principal component

Future extraction

One can also use PCA to extract important information:

Data clustering

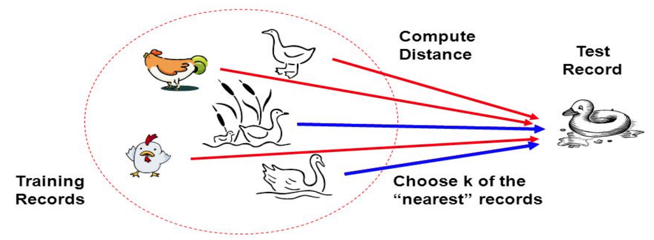
How to divide the data into groups? (i.e. how to cluster the data?)



Not easy in high dimensions.

Species classification

One can use data clustering to classify species.



> *"If it walks like a duck, quacks like a duck, and looks like a duck, then it's probably a duck."*

We have some known clustered (by features) data. Compare the new one with existing clusters.

Other potential applications of data clustering:

- identifying biological properties;
- classifying credit card transactions;
- categorizing documents (e.g. novel, politics, etc.).

iOS/Andriod:
PlantNet

“Pl@ntNet is an application that allows you to identify plants simply by photographing them with your smartphone...”

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Simulation modeling

In empirical modeling, one needs data.

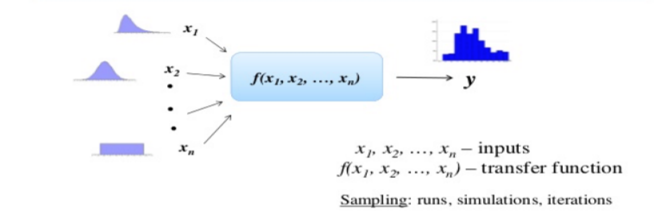
There are situations where experiments are expensive, or even impossible.

- It is harmful to inject certain drugs in body.
- Tests are expensive in the design of aircraft.

Therefore, one needs to simulate the situation. That is, we use random numbers to simulate the appearance of certain events.

We will discuss the basic idea of Monte Carlo simulations.

Monte Carlo simulations



- The inputs are modeled by random numbers (with various distributions).
- The output y is computed by f (which is also a random variable).
- One obtains f by some knowledge such as measurement data.

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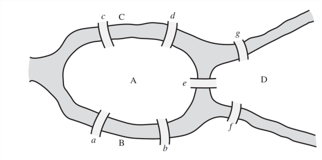
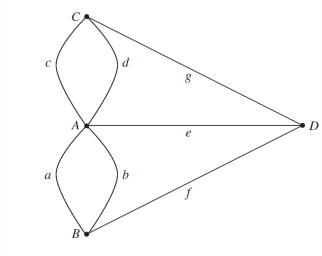
Modeling by graph theory

Some problems can be modeled by graphs.

A graph G contains 2 sets: a vertex set $V(G)$ & an edge set $E(G)$.





Seven Bridges of Königsberg

Example 1: Social network

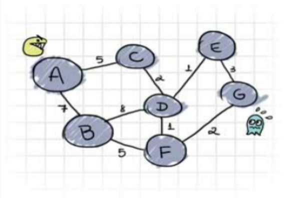
A social network can be modeled by a graph:

- Each user is considered as a vertex.
- Two users can form an edge if they are friends.
- One interesting problem is the degree of separation, it is the shortest distance between any 2 users.
- In 2016, the average degree of separation of Facebook users is 4.57.

Example 2: Route planning

Route planning problem can be modeled by a graph:

- Each road intersection is considered as a vertex.
- A road between two adjacent intersections is an edge.
- The problem is to find a path giving the shortest distance between 2 destinations.
- We see that there is a need to give weights to edges.



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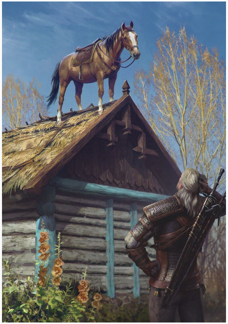

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Optimization modeling

We consider optimization problems: find X^* such that

$$f(X) \quad \text{is optimized,}$$

where $X = (x_1, \cdots, x_n)$ are called decision variables.

- Unconstrained: f is optimized without restrictions on X.
- Constrained: there are restrictions on X.
  - Equalities: $g_i(X) = b_i$, for $i = 1, 2, \cdots, m$.
  - Inequalities: $g_i(X) \leq b_i$, for $i = 1, 2, \cdots, m$.
  - Mixed: both equalities and inequalities.

Example

Find X^* such that

$$f(X) \quad \text{is optimized}$$
$$\text{subject to} \quad g_i(X) = b_i \text{ or } g_i(X) \leq b_i$$

- f can be profit to be maximized, g_i are some resource limitations.
- f can be the risk to be minimized, g_i are expected earnings.

Classifications

- f and g_i are linear. This is linear programming.
- f and g_i are linear and X integer. This is integer programming.
- f and g_i is/are nonlinear. This is non-linear programming.

Example: integer programming

Suppose:

- net profits of \$25 per table, and \$30 per bookcase;
- the carpenter has 690 units of wood, and 120 units of labor;
- each table requires 20 units of wood and 5 units of labor;
- each bookcase requires 30 units of wood and 4 units of labor.

We can then formulate the following

$$\text{maximize} \quad 25x_1 + 30x_2$$

subjects to

$$20x_1 + 30x_2 \leq 690,$$
$$5x_1 + 4x_2 \leq 120,$$

where $x_1 \geq 0$, $x_2 \geq 0$ and x_1, x_2 are integers.

Example: portfolio optimization

Suppose that there are n assets. You want to invest a fixed amount of money. How do you allocate your investments?

Let x_i be the portion of money invested in the asset i.

Two important factors: return and risk

- Assume μ_i is the average return of asset i. On average, you have the following return

$$\mu_1 x_1 + \mu_2 x_2 + \cdots + \mu_n x_n$$

- Risk is typically modeled by a $n \times n$ positive definite matrix Q. The risk is

$$\frac{1}{2} x^T Q x$$

where $x = (x_1, x_2, \cdots, x_n)^T$. Risk is large if this number is big.

Two common ways

- We find x_i so that

$$\text{maximize} \quad \mu_1 x_1 + \cdots + \mu_n x_n - \frac{1}{2} x^T Q x$$

(maximize return at the same time minimize risk) subjects to

$$x_1 + \cdots + x_n = 1, \quad x_i \geq 0.$$

- Given a fixed number R, we find x_i

$$\text{maximize} - \frac{1}{2} x^T Q x$$

subjects to

$$x_1 + \cdots + x_n = 1, \quad x_i \geq 0$$

and

$$\mu_1 x_1 + \cdots + \mu_n x_n \geq R$$

(minimize risk, and having return of at least R).

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Modeling with differential equations

Modeling quantities that change continuously in time (For example, populations, concentration of chemicals, etc.).

(Recall that, difference equations model quantifies that change in discrete time intervals.)

A differential equation is an equation relating a quantity of interest and its derivatives, e.g.,

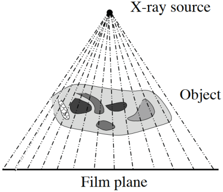
$$\frac{\mathrm{d}x}{\mathrm{d}t} = ax(b-x), \quad \frac{\mathrm{d}^2y}{\mathrm{d}t^2} + 2t\frac{\mathrm{d}y}{\mathrm{d}t} = 3y.$$

Derivatives represent instantaneous change rates of a quantity.

A mathematical problem

Can one determine the internal properties of a medium by making measurements outside the medium?

(a) A old-fashioned chest x-ray image. (Image provided courtesy of Dr. David S. Feigin, ENS Sherri Rudinsky, and Dr. James G. Smirniotopoulos of the Uniformed Services University of the Health Sciences, Dept. of Radiology, Bethesda, MD.)



(b) Depth information is lost in a projection.

Q: Can we determine internal properties from attenuation of X-rays?

Attenuation coefficient

Attenuation coefficient—$\mu(x)$ quantifies the tendency of an object to absorb X-rays.

Material	**Attenuation coefficient in Hounsfield units**
water	0
air	−1000
bone	1086
blood	53
fat	−61
brain white/gray	−4
breast tissue	9
muscle	41
soft tissue	51

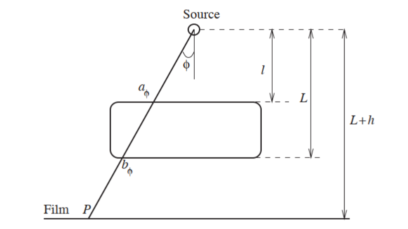
(Don't worry about the negative signs.)

Beer's law

Beer's law states that the intensity of X-ray—$I(s)$ satisfies

$$\frac{\mathrm{d}I}{\mathrm{d}s} = -\mu(s)I(s),$$

where s is the arc-length parameter along the X-ray.



Example: Drug dosage

We combine differential and difference equations in a model.

Q: How can the doses and the time between doses be adjusted to maintain a safe but effective concentration of drug?

Assumption 1: Decay of drug

Let $C(t)$ be the concentration of the drug. Then we assume

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -kC$$

where $k > 0$ is the decay rate.

Assumption 2: Constant dosage

A dose of C_0 is added at fixed time intervals of length T.

Example: the SIR model

$S(t) =$ the number of susceptible population,
$I(t) =$ the number of infected population,
$R(t) =$ the number of removed population
(either by death or recovery),
$N =$ the number of total population.

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\frac{\beta IS}{N},$$
$$\frac{\mathrm{d}I}{\mathrm{d}t} = \frac{\beta IS}{N} - \gamma I,$$
$$\frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I.$$

This is a simplified model and is also far from the reality (vaccination, the possibility of re-infection, incubation, etc.).

Finding solutions

We will discuss three ways to find solutions:

- analytical solutions, but only for simple cases;
- graphical solutions, may work for a more general class of differential equations to understand qualitative behaviors including long term behaviors;
- numerical solutions, can work for almost all cases, and one can obtain approximate values of solutions.

Course webpage

https://www.math.cuhk.edu.hk/course/2324/math3290

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