MATHEMATICAL MODELING AND SIMULATION

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Abstract. We propose a few specific mathematical modeling techniques at graduate level used in various applications such as reliability engineering, biomathematics. These are aimed for graduates in Applied Mathematics and CS at HCMUT.

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The aims the course

This lecture integrates mathematical and computing techniques into modeling and simulating of industrial and biological processes.

The structure of the course. The course consists of three parts:

Part I: Introductory specific topics

Part II: Methods and Tools

Part III: Connections and research projects

Part I: Introductory specific topics – case studies

- MM and Simulation: mathematical models for simulation, why?
- MM and Simulation: mathematical models for simulation, how?
- An Ecological System: could you? A basic tool in simulation.
- An Economic System: a practical demand in .
- A Biological Phenomenon: a multipurpose tool from .

Part II: Methods of MM and Simulation

We will discuss the followings:

- Introductory Simulation
- Dynamic Systems
- Computer-aided modeling
- Probabilistic and stochastic techniques
Part III: New applications of MMS

We investigate two fascinating following applications:

- Probabilistic Modeling
- Statistical Modeling
- Numerical Modeling: canceled
- Biological Modeling: postponed this semester
- Epidemic Modeling: postponed this semester

Working method.

Each graduate is expected to carry out a small independent research project (max 20 pages, font size 10, 1.5 line spacing, Time new roman) from the above topics and submit his (her) report at the end of the course.
1. PART I: MOTIVATED TOPICS OF MMS

1.1. Mathematical modeling and simulation Why?

- Increasing the understanding of the system,
- Predicting the future system behavior,
- Carrying technical and quantitative computations for control design, from which optimization can be done
- Studying human-machine cooperation.

1.2. Mathematical modeling and simulation How?

The modeling process itself is (or should be) most often an iterative process: one can distinguish in it a number of rather separate steps which usually must be repeated. One begins with the real system under investigation and pursues the following sequence of steps:

(i) empirical observations, experiments, and data collection;

(ii) formalization of properties, relationships and mechanisms which result in a biological or physical model (e.g., mechanisms, biochemical reactions, etc., in a metabolic pathway model; stress-strain, pressure-force relationships in mechanics; functional relationships between cost and reliabilities of distinct components in a software development projects);

(iii) abstraction or mathematization resulting in a mathematical model (e.g., algebraic and/or differential equations with constraints and initial and/or boundary conditions);

(iv) model analysis (which can consist of simulation studies, analytical and qualitative analysis including stability analysis, and use of mathematical techniques such as perturbation studies);

(v) interpretation and comparison (with the real system) of the conclusions, predictions and conjectures obtained from step (iv);

(vi) changes in understanding of mechanisms, etc., in the real system.

1.3. Cautions. Common difficulties and limitations often encountered in the modeling of systems:

(a) Availability and accuracy of data; (b) Analysis of the mathematical model;
(c) Use of local representations that are invalid for the overall system;
(d) Assumptions that the ‘model’ is the real system;
(e) Obsession with the solution stage; (f) Communication in interdisciplinary efforts.
1.4. **Typical applications.**

*Finance Trend Analysis* with *Stochastic Calculus*.

*An Industrial Manufacturing System*- Car production with Computational Algebra.

*A Financial Model in Economics*- Black-Scholes model in Finance.

*A Biological Phenomenon*.

1.5. **Computing Software.**

Introduce *SciLab, OpenModelica*, **G.A.P**, *Singular, Maple* and so on.
Part II: Techniques and Algorithms.
2. Dynamic Systems

2.1. Introductory Dynamic Systems. We outline the modeling process of dynamic systems and introduce major tools of the trade. Our viewpoints are:

- connection between models and data – namely connection between dynamic modeling and statistical modeling, is the first concern, and
- modern computer-based statistical methods must be applied intensively to dynamic models.

Connecting models with data is almost always the eventual goal. So taking the time to learn statistical theory and discrete methods will make you a better modeler and a more effective collaborator with experimentalists.

2.2. Discrete Dynamic Systems- a case study.

Consider a simple discrete dynamic system $S$ that depends on four binary variables $f, g, c, w$. [$S$ changes its states when $f, g, c, w$ change their values.] Suppose that

- only $f$ is the factor that can change states of $S$, i.e. state $u$ changes to another state $v$ if and only if the equality $u_f + v_f = 1$ holds
- a state $u = (u_f, u_g, u_c, u_w)$ changes to another state $v = (v_f, v_g, v_c, v_w)$ iff at most two coordinates of them are different,
- the system evolves from the initial state $s_I = (0000)$ (source) to a final state $s_F = (1111)$ (sink).

The aim: provided some constraints between the four binary variables, we want to choose a shortest path from the source $s_I = (0000)$ to the sink $s_F = (1111)$.

2.2.1. Tools- Techniques.

Definition 1 (Brute-force). Search exhaustively all possibilities of the search space and, after checking, list all solutions.

Obviously all possible states $V$ of the system $S$ above are the solution set of the polynomial system of equations

\[ f^2 - f = g^2 - g = c^2 - c = w^2 - w = 0. \]
However, if no constraint is detected and imposed, you have to search exhaustively all possible paths from $s_I$ to $s_F$: this task is computationally impossible when we have a lot binary variables or their values are not binary. For instance, if we use

**Constraint I:**

$$(I_a)\ f, g \text{ and } c \text{ must receive the same value } a \in \{0, 1\}$$

$$(I_b) \text{ OR } \ g \text{ and } c \text{ must receive different values}$$

then a few states must be discarded from $V$, such as $\{(1, 0, 0, 1), (0, 1, 1, 0)\}$.

**Definition 2 (State-transition graph).** State-transition graph $G = (V, E)$ of a developing system $S$ is a directed graph where

- the vertices $V$ consists of all feasible states that the system can realize
- the edges $E$ consists of arcs $e = (u, v)$ such that state $u$ can reach to state $v$ during the evolution of the concerned system

In our specific example above, $V$ can hold all $16 = 2^4$ possible states if no system invariants would be found and imposed on $S$. With Constraint I, $V$ can be redefined as $V := V \setminus \{(1, 0, 0, 1), (0, 1, 1, 0)\}$.

**Definition 3 (System invariants).** Invariants of the system $S$ are specific constraints or properties that do not change when the system factors (variables) change their values [to ensure $S$’ stability, existence …] during the evolution of concerned system.

For instance, if we require that

(i) either $f, g$ and $c$ must receive the same value $v \in \{0, 1\}$

(ii) or $g$ and $c$ can not receive the same value $v \in \{0, 1\}$ if $f$ gets value $1 - v$

what would be the invariants you could say?

In case (i), easy to formulate the first invariant $f = g = c$.

**Definition 4 (Hamming distance).** The Hamming distance $d(u, v)$ between two binary states $u = (u_1, u_2, u_3, u_4)$ and $v = (v_1, v_2, v_3, v_4)$ is the number of their distinct coordinates:

$$d(u, v) = |u_1v_1| + |u_2v_2| + |u_3v_3| + |u_4v_4|$$
2.2.2. Solution.

2.3. Continuous Dynamic Systems. Major steps are:

1. Setting the objective
2. Building an initial model
3. Developing equations for process rates
4. Nonlinear rates from data: nonparametric models
5. Stochastic models
6. Fitting rate equations by calibration

2.3.1. Setting the objective. Few crucial steps should be considered in this phase:

- Decide the objective to be theoretical or practical modeling; where
  - theoretical modeling: the putative model helps us to understand the system and interpret observations of its behavior
  - practical modeling: the putative model helps us to predict the system
- Decide how much numerical accuracy you need
- Assess the feasibility of your goals: should a bit pessimism (start small first, and then expand it to a more complex one)
- Assess the feasibility of your data: should a bit optimistic (don’t worry if you miss some data from the beginning)

2.3.2. Building an initial model.

Conceptual model and diagram. The best known is compartmental model; you have to decide which variables and processes in the system are the most important and which compartment should they be located.

2.3.3. Developing equations for process rates. Having drawn a model diagram, we next need an equation for each process rate. Mathematically, we need a differential equation expressed by:

- an Ordinary Differential Equation (ODE) of the form:

\[ \dot{x} = f(x, u, t) \]

where \( \dot{x} \) denotes the derivative of \( x \) (the state variables) with respect to the time variable \( t \), and \( u \) the input vector variable, or
by Differential Algebraic Equations (DAE):

\[
\begin{aligned}
x' &= f(x, u, t) \\
0 &= g(x, u, t)
\end{aligned}
\]

Linear rates: when and why?.

Nonlinear rates from data: fitting parametric models.

Nonlinear rates from data: selecting a parametric model.

Cross validation, a computational approach

2.3.4. Nonlinear rates from data: nonparametric models. Multivariate rate equations.

2.3.5. Stochastic models.

2.3.6. Fitting rate equations by calibration.

2.3.7. Summary.
3. **Computer-aided modeling**

3.1. *Computer Algebra and Applications in Modeling.*

3.2. *Algebraic Modeling.*

3.3. *Bond Graphs and Usages.*
4. Simulation

4.1. Introductory Simulation.

4.2. Scaling or Dimensional analysis.

4.3. Block diagrams.

4.4. Connecting subsystems.

4.5. Simulation languages.


4.7. Model Validation.
5. Probabilistic and stochastic techniques

We will discuss the followings:

- Generating Functions
- Branching processes
- Markov processes
- Birth and Death processes
- Multi-dimensional processes
- Multi-type branching processes
Part III: New applications of MMS.
6. Probabilistic Modeling for Finance

Main references:

1/ Chapter 6 of *Simulation, A Modeler’s Approach* by Jame Thomson, Wiley, 2000

2/ Chapters 1, 2 of *Introduction to the Mathematics of Finance* by Ruth J. Williams, AMS vol 72, 2006


6.1. **Introduction**— A problem in Finance. Observing fluctuations in financial market and making inference

6.2. **How to make a math model?**— Binomial Model.

6.3. **How to solve it?** The role of Stochastic Processes and Calculus.

6.4. **ITO’s lemma.**
7. **Statistical Modeling 1—DOE for SQC**

Main references:

The Application of Computational Algebraic Geometry to the Analysis of Design of Experiments: A Case Study, by Holliday, Pistone, Riccomagno, Wynn,

7.1. **A problem in Statistical Quality Control.**

7.2. **How to make an experiment design?**

7.3. **How to measure factor interactions?**

7.4. **What should we do to bring experiments into daily life?**
8. **Statistical Modeling 2– Black-Scholes model in Finance**

Main references:

2/ Chapters 3 of *Introduction to the Mathematics of Finance* by Ruth J. Williams, AMS vol 72, 2006

3/ Chapter 2, 5, 6 of

8.1. **Finite market model.**

8.2. **Making economic decisions under uncertainty.**

9. **Conclusion**

**References**


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<td>Working areas</td>
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