## Methodology for Computer Science Research Lecture 4: Mathematical Modeling

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## - Definitions and Goals

- Building blocks
- Model types
- Model evaluations
- A set of Model Classes
- Examples


## What is Mathematical model?

A researcher wants to study a real physical system, but (s)he cannot due to a set of limitations (be it money, knowledge, or complexity).
In that case mathematical modeling (or shortly, modeling) is used.

Modeling as a process is a transformation of knowledge from reality to a model space. That transformation is always happens with accuracy losses (they are called assumptions), otherwise there is no need for model.

Mathematical model is a mathematical definition of a system, which is formed as a formal idealization or modeling (under a set of assumptions) of the original system.

## Aims of modeling

With formal mathematical model constructed, it is possible to:

- Study properties of the system, which is hard to get in reality.
- Idealize and omit unknown properties.
- Predict future/asymptotic behavior of the system.
- Optimize a real system, based on optimization criteria of the model.
- Verify (with some probability) relations between parameters (black-box model).
- Substitute expensive (or complex) study of the real system for a cheap evaluation of model system (i.e., if somebody constructed and verified a model, then it can "easily" be reused).


## Modeling

The process of construction a mathematical model based on real physical system is modeling.

The mathematical model is not unique for a given system but it is uniquely defined by transformation process (modeling).

Producing a model one should remember what is the set of assumptions was used (these idealizations are the most important parts of the modeling process). Potentially they are the sources of errors/inaccuracies.

## Assumptions and model preference diagram

As it was said, the modeling process is always accompanied with accuracy losses. It is always possible to construct inaccurate model.


Almost all models form a series of trade-offs between assumptions (inaccuracy) and evaluation complexity.

## Relations to the reality

Mathematical model can be used, only when it is "sufficiently" accurate!!!


Otherwise the results of computations on models cannot be adopted, i.e., there is not connections between modeling results and practical results.

## Domains of model usage

Models are created under set of assumptions, which define the domain of usage. They are evaluated inside such domain, and thus with some percentage accurate only inside of the domain. Accuracy outside cannot be expected.


Examples:

- Domain A - Saturated model (all stations have something to send); domain B - unsaturated model; domain $A \bigcap B$ is empty.
- Domain $A$ - queue size $\geq 1$; domain $B$ - queue size $<100$; domain $A \cap B$ is queue size $(1,100)$.
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## Building blocks for Models

Mathematical models consist of

- Variables
- Relations

Modeling processes do

- define "independent", "dependent" and "partially dependent" events occurrence as variables;
- connect dependence between events as relations;
- omits explicit introduction of variables for rare or insignificant events (if not needed);
- simplifies relations between variables, whenever possible.


## Variables (1/2)

Variables:

1. Decision variables $u$ (or control, independent variables).

Controllable by the decision makers.
2. Input variables.

Input to the system $\lambda$, which the decision makers cannot control.
3. Exogenous variables $\alpha$ (parameters, constants).

Parameters that comes from outside the model and are a priori given to the model.

## Variables (2/2)

Variables:
4. Random variables $\zeta$.

Some unknown (stochastic) influence to the system outside, or through complex internal structure.
5. Output variables $\mu$.

Output from the system, based on the state of the model (state variables).
6. State variables $x=x(u, \lambda, \zeta, \alpha)$.

State of the system, which is produced by influence of decision, input, random, exogenous variables.

## Examples of variables

1. Decision variables - request download $u$ bytes; forward message to a node $A$ or $B$.
2. Input variables - input rate to the system $\lambda_{1}, \lambda_{2}, \ldots$; a new packet comes every second.
3. Exogenous variables — download/upload speed; SNR (signal-to-noise ratio); speed of the light.
4. Random variables - radio noise (some distribution); inter-arrival time (e.g., Poisson process).
5. Output variables - sent messages without response; atmosphere heating.
6. State variable - current energy of device (can be calculated by initial energy, and spent energy); coordinate of a moving object (initial coordinate and velocities); size of the queue (calculated based on initial size, input process, time elapsed, etc...).

## Variables' relations

Functions that connects different variables together:

1. Constraints

$$
g_{i}(x) \leq 0, i=1,2, \ldots, l
$$

where $I$ is number of constraints, $x=x(u, \lambda, \zeta, \alpha)$. Note, no need for $g_{i}(x)=0$, it is result of $g_{i}(x) \leq 0$ and $h_{i}(x)=-g_{i}(x) \leq 0$.
2. Objectives

$$
\underset{u \in U}{\operatorname{minimize}}\left\{f_{1}(x), f_{2}(x), \ldots, f_{j}(x)\right\}
$$

where $x=x(u, \lambda, \zeta, \alpha)$.

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## Model types

1. linear vs. non-linear
2. deterministic vs. probabilistic
3. static vs. dynamic
4. discrete vs. continuous
5. lumped vs. distributed
6. structured vs. functional

## Model types: linear vs. non-linear

If operators (constraints and/or objectives) are linear then the model is linear, otherwise it is non-linear.

An example of linear operator $f(x)=a \cdot x+b$.
Linear regression is sometimes studied for two random variables, i.e. if $X, Y$ random variable, then is it possible to find $a, b$ such that $Y=a \cdot X+b$ with high probability. Existence of linear regression means that there is dependence between the variables.


An example of non-linear operator $f(x)=x^{2}-x$.
Optimization objective functions if they are not trivial are always non-linear functions (in case of linear objectives solution is always one of the bounds).

## Model types: deterministic vs. probabilistic

In deterministic models, the state variables are uniquely defined by initial parameters of the model.

An example, a connection between speed, distance and time:

$$
\text { Speed }=\frac{\text { Distance }}{\text { Time }} .
$$

In probabilistic models, the state variables are not uniquely defined by initial parameters, they are defined by probability distributions.
An example, random walk on whole axis:

$$
\text { position }(t+1)= \begin{cases}\operatorname{position}(t)+1, & \text { with probability } \frac{1}{2} \\ \operatorname{position}(t)-1, & \text { with probability } \frac{1}{2}\end{cases}
$$

## Model types: deterministic vs. probabilistic

An example of random walk on 2D lattice ${ }^{1}$

${ }^{1}$ From http://mathworld.wolfram.com/RandomWalk2-Dimensional.html

## Model types: static vs. dynamic



Static models do not consider time influence, while dynamic does.

Static state, does not change with time, i.e. $x=c$.

Static models mainly study properties of parameters, i.e. how some parameters depend on the initial values of other parameters.

Dynamic state does change with time, i.e. $x=x(t)$.
Dynamic often study system as differential equations, i.e. future value depends on the value before and a set of other variables (including control in case of control theory or game theory).

## Model types: discrete vs. continuous

Discrete models:

$$
\begin{aligned}
x_{n+1} & =f\left(x_{n}\right), \text { if } n \geq 1 \\
x_{0} & =c .
\end{aligned}
$$



Continuous models:

$$
\begin{aligned}
\dot{x}(t) & =f(x(t)), \text { if } t>0 \\
x(0) & =c .
\end{aligned}
$$

Examples from http://mathworld.wolfram.com/RandomWalk2Dimensional.html.

## Model types: structured vs. functional

Also known as, white-box vs. black-box.

- Structured (or white-box), given the whole structure of the model, it is required to study the variable properties.
- Functional (or black-box), given a set of inputs and set of outputs, the internals of the system are not known, it is require to find some dependencies between variables (with limited knowledge).


## Mathematical model usage: direct and opposite

- Direct - we know the structure and all connections inside model, we need to retrieve additional useful information about the model.
An example: we know the sending rate, delay, congestion, and so on; we need to get throughput rate.
- Opposite - we know a set of possible models, we need to select one concrete model based on additional data. An example: we know what behavior we want from the system, we would like to construct set of parameters which achieve it (in Game Theory it is called Mechanism Design).
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## Conceptual model

First construction - conceptual model.
Whenever researcher is starting modeling process, there is no information about what model should be constructed, what should be omitted or simplified and what should be explicitly described in the model.

This first task is the task of concept construction, the starting point of modeling, or even extension of the model to a new levels.

It is also called, mental model, or premodel.
The creation of the conceptual model may be simplified if the field already has these models available, and researcher do not have to start from the scratch.

## Construction of conceptual models

- Hypothesis ("that could be"). Trial to define an event.
- Phenomenological model ("consider as if it is true").
- Approximation ("consider something too big or too small").
- Assumptions ("omitting something for simplicity/clearance").
- Heuristic model ("there is no prove of it, but it let us study deeper").
- Analogy ("consider only some specific features").
- Thought experiment ("proof by contradiction").
- Demonstration of possibility ("show that it does not contradict to possibility").


## Formal model

Formal model is produced later during study.
Formal model, is concept opposite to the conceptual model or premodel. It is final model, or mathematical model, which was studied and verified using different methods.

Formal model, may be extended further using new conceptual model, however, formal by itself is considered to be self-sufficient well-studied model with sufficient accuracy.

## Conceptual model to formal model

To move model "status" from the conceptual to the formal or discarding model. It should be

- Verified, or
- Falsified (for discarding).

The verification of the model depends on the model and the complexity of analysis.

Whenever we falsify a model, we cannot use it anymore as accurate, however the verification does not guarantee that the model is really accurate. It gives that with certain probability it is a valid model (was tested and validated in some environment).

## Model accuracy verification

- Empirical data. In order to verify model with a given empirical data, divide the data onto two sets:

1. Train data - to train the model.
2. Verification data - to verify.

Verification is done by "measuring" distance between predicted parameters and verification data.
Statistical models also may be used here.

- Applicability. Based on the training data, and physical system the model cannot predict something that was not yet seen in physical model (and documented) in real system. This is a limitation of the model, or applicability.


## Types:

- interpolation - does the model describes well the properties of the system between data points,
- extrapolation - does the model describes well the properties of the system outside data points.
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## Simple parametric model

Simple connections between essential variables, such as

$$
x=\lambda r t
$$

where $t$ is time, $r$ is rate, and $\lambda$ some parameter. Furthermore, we may find

$$
r=\frac{\gamma}{\beta}
$$

and then conclude

$$
x=\lambda \frac{\gamma}{\beta} t
$$

## Markov chains

Markov chains model is one of the most popular Probability models. It has intuitive visual form.


Given random variable $X$, every state is possible value for the random variable. Transitions happen during one unit of time. $P_{i}(t)$ is the probability to do in state $i$ at time $t, P_{i, j}=P(j \mid i)$ - is conditional probability to be in state $j$, after state $i$, also transition probabilities.

It has very important Markov property - future is independent from the past given current.

## Markov chains



If Markov chain is ergodic, i.e., every state can be reached from every state and aperiodic, then there exists steady state $\pi$.
If transition matrix is

$$
P=\left(\begin{array}{lll}
p_{11} & p_{12} & p_{13}  \tag{1}\\
p_{21} & p_{22} & p_{23} \\
p_{31} & p_{32} & p_{33}
\end{array}\right)
$$

then $\pi=\pi \cdot P$.
One step on the Markov chain is equivalent to multiplication by the matrix $P$. If network is ergodic then any initial distribution $\pi_{0}$ every step converges to steady state $\pi$.

## Bayesian networks

When we have a set of random variables, and do not know the connection between them. Bayesian belief propagation model helps:


Opposed to Markov chain the states are not value of one random variable, but different random variables itself. The connections are directed acyclic graphs (DAGs).

$$
\begin{aligned}
& P(R) \\
& P(S)=P(S \mid R) P(R) \\
& P(G)=P(G \mid S, R) P(S \mid R) P(R)
\end{aligned}
$$

## Optimization models

In optimization models, we are to optimize an objective, under set of constraints
$J=\int_{0}^{T} g(x, u, s, t) d t \rightarrow \underset{u}{\max ,}$

$$
\dot{x}(t)=f(x, u, s, t),
$$

$$
I(x, u, t) \leq 0,
$$

$$
\begin{aligned}
& J=\sum_{i=0}^{N} g_{i}(x, u, s) \underset{u}{\rightarrow} \max , \\
& x_{i+1}(t)=x_{i}+f_{i}(x, u, s), \forall i, \\
& I(x, u) \leq 0, \\
& u \in U .
\end{aligned}
$$

$u \in U$,
An example:

$$
\begin{aligned}
& J=x y \rightarrow \max , \\
& x^{2}+y^{2} \leq 10, \\
& x, y \in \mathbb{Z} .
\end{aligned}
$$

Objective can be money, efforts, distance, time, and so on, whatever we want to maximize (minimize).

## Optimization models

Optimization problems sometimes are non-trivial.


Derivative does not necessary shows needed optimums (it shows only local optimums) additional study often is needed.

## Game theory

Formulated similiar way as the optimization models:

$$
\begin{aligned}
\int_{0}^{T} g(x, u, s, t) d t \underset{u_{1}}{\vec{u}} \max , & \quad \int_{0}^{T} g(x, u, s, t) d t \rightarrow \underset{u_{2}}{ } \max \\
\dot{x}(t) & =f(x, u, s, t) \\
I(x, u, t) & \leq 0 \\
u & \in U
\end{aligned}
$$

However, we have multi-optimization problem. Every "player" has own objective function, which it wants to optimize. "Conflict" happens in the trajectory equations $\dot{x}(t)=f(x, u, s, t)$.

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## An Example: Queueing discipline

Classical example:


- Server has the average service time $\mu$.
- Input rate (average) is $\lambda$.
- Depending on how fast server processes message the queue size grows or reduces.
- Stability (long-term) is achieved if $\lambda<\mu$.

Little's law: Let $L$ is average number of customers, $\lambda$ is arrival time and $W$ average waiting time for a customer, then

$$
L=\lambda \cdot W \text {. }
$$

## An Example: Transport protocol

A well-known TCP equation:
$B(p) \approx \min \left(\frac{W_{\max }}{R T T}, \frac{1}{R T T \sqrt{\frac{2 b p}{3}}+T_{0} \min \left(1,3 \sqrt{\frac{3 b p}{8}}\right) p\left(1+32 p^{2}\right)}\right)$,
where $B(p)$ is the throughput of the TCP connection, $p$ is the loss probability, RTT is the average round trip time, $W_{\max }$ is maximal congestion control window, and $b$ is the number of packets that are acknowledged by received ACK packet (often $b=2$ ).

Padhye, J., Firoiu, V., Towsley, D., and Kurose, J. 1998. Modeling TCP throughput: a simple model and its empirical validation. SIGCOMM Comput. Commun. Rev. 28, 4 (Oct. 1998), 303-314.

## An Example: Backoff protocol



Average service time:

$$
E S=\frac{1}{\left(1-p_{c}\right)\left(1-\left(1-p_{c}\right)^{\frac{1}{N-1}}\right)}
$$

where $p_{c}$ is collision probability in the network. Optimal point (minimal service time):

$$
p_{c}^{*}=1-\left(1-\frac{1}{N}\right)^{N-1}
$$

## Computer systems that help

- Maple,
- Mathematica,
- Mathcad,
- MATLAB,
- VisSim.

