OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

INF FAKULTÄT FÜR INFORMATIK

Introduction to Simulation

Markov Chains

Contents

Contents of the lecture

Motivation

We want to build models that aid medical diagnoses.

Motivation

The situation:

- We do not know which disease a patient has.
- We have a stochastic model of each disease.
- The disease has different stages.
- We know the daily probability of each state transition.
- We know the probability of each measurement at each stage.
- We can measure different symptoms.

We want to determine which disease is more likely.

But ...

- we cannot directly observe the progress of the disease.

Markov Chains

A Markov chain is a stochastic process …

- with discrete states,
- with state changes at discrete points in time.

For any pair of states, …

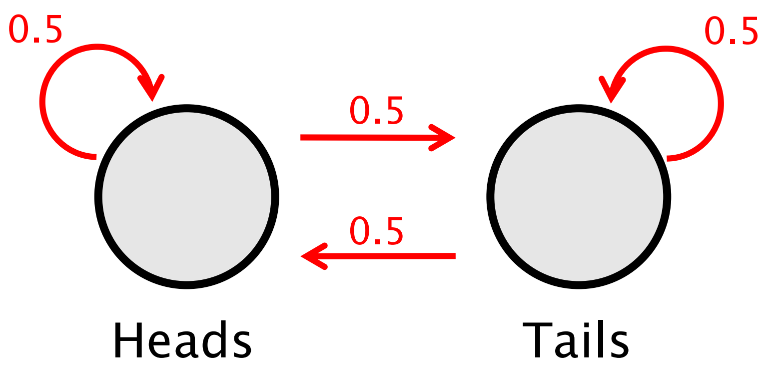
- the state change between them has a fixed probability.

Markov chain representations:

- Mathematically: Using linear algebra notation
- Graphically: As a directed, annotated graph

A Very Simple Markov Chain

Repeated coin tossing



Mathematical Representation

Matrix P:

$$P = \begin{bmatrix} p_{hh} & p_{ht} \\ p_{th} & p_{tt} \end{bmatrix} = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

Solution vector π:

$$\pi = (\pi_{Heads}, \pi_{Tails})$$

Properties:

- P is a stochastic matrix.
- π is a probability row vector.

Mathematical Representation

Solving the Markov chain:

- Iterated matrix–vector multiplication

$$\pi_k = \pi_{k-1} \cdot P$$

Example for coin tossing (Assume first result is *Heads*)

$$\begin{aligned}
\pi_1 &= (1.0, 0.0) \\
\pi_2 &= (0.5, 0.5) \\
\pi_3 &= (0.5,\ 0.5) \\
&\vdots
\end{aligned}$$

A Slightly More Interesting Example

Where does Graham go to eat every evening?

- Three restaurants: Italian (I), Greek (G), Chinese (C)

Observe Graham for 300 days:

- C G I I C G C I C C G G C I C G I C G C G I I C G C G C I G C …

Count # occurrences of each choice:

	C	G	I
C	20	30	50
G	10	30	60
I	30	40	30

A Slightly More Interesting Example

Solution vector: $\pi = (\pi_C,\ \pi_G,\ \pi_I)$

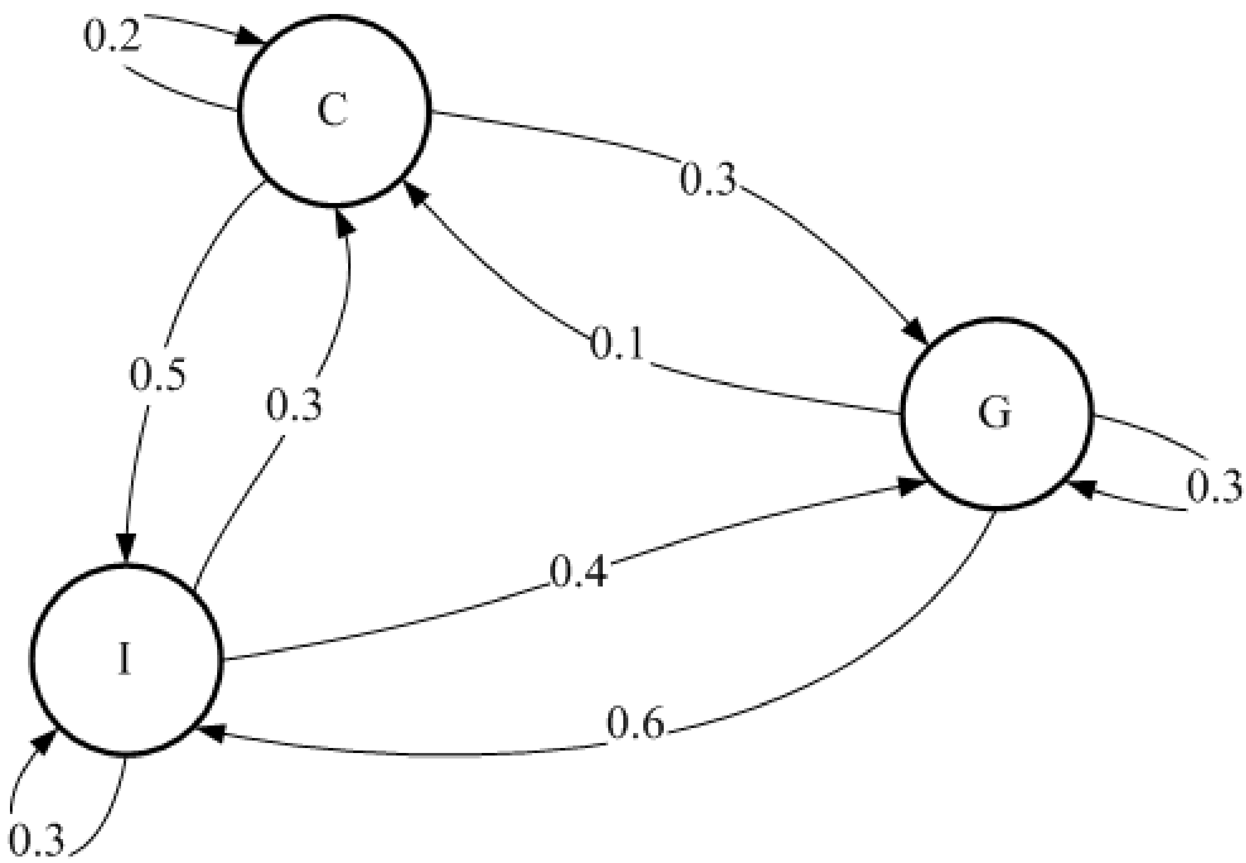
Stochastic matrix: $$P = \begin{bmatrix} p_{CC} & p_{CG} & p_{CI} \\ p_{GC} & p_{GG} & p_{GI} \\ p_{IC} & p_{IG} & p_{II} \end{bmatrix} = \begin{bmatrix} 0.2 & 0.3 & 0.5 \\ 0.1 & 0.3 & 0.6 \\ 0.3 & 0.4 & 0.3 \end{bmatrix}$$

Solution (assuming first meal was C):

$$\begin{aligned}
\pi_0 &= (1.0000\quad 0.0000\quad 0.0000)\\
\pi_1 &= (0.2000\quad 0.3000\quad 0.5000)\\
\pi_2 &= (0.2200\quad 0.3500\quad 0.4300)\\
\pi_3 &= (0.2080\quad 0.3430\quad 0.4490)\\
\pi_4 &= (0.2106\quad 0.3449\quad 0.4445)\\
\pi_5 &= (0.2100\quad 0.3445\quad 0.4456)\\
\pi_6 &= (0.2101\quad 0.3446\quad 0.4453)\\
\pi_7 &= (0.2101\quad 0.3445\quad 0.4454)\\
\pi_8 &= (0.2101\quad 0.3445\quad 0.4454)
\end{aligned}$$

A Slightly More Interesting Example

Graphical representation of the Markov chain:



Applications

Markov chains are extremely widespread.

They are used in many fields of Science, for example:

- Physics (thermodynamics, mechanics)
- Chemistry (growth of molecules, enzyme behaviour)
- Informatics (data compression, pattern recognition)
- Operations Research (queues, logistics)
- Economics (market behaviour, pricing models)
- Biology (population dynamics)
- Medicine (epidemiology)

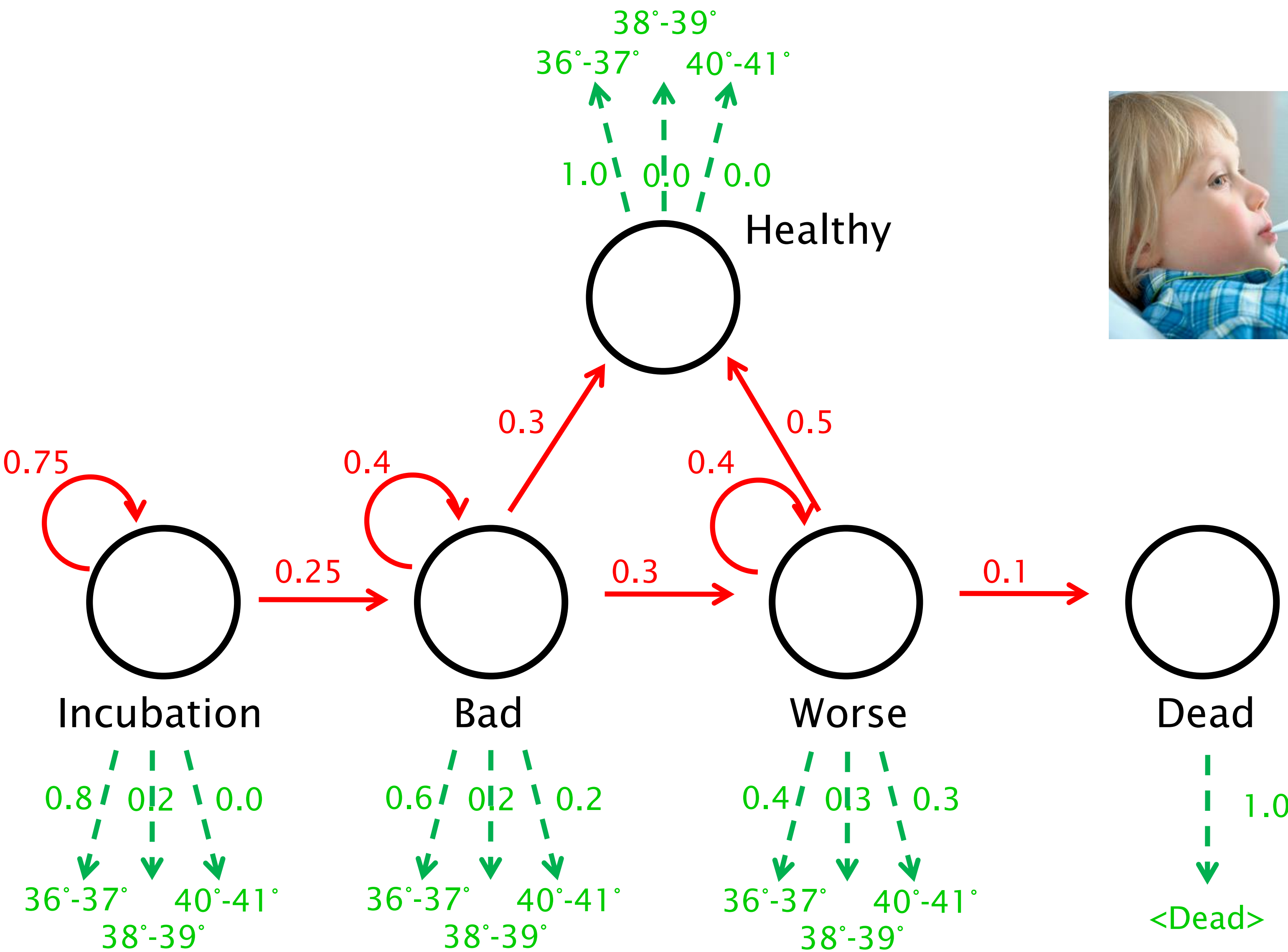
Example

The situation to be modelled:

- The patient has either disease A or disease B.
- We can take their temperature once per day.
- We have a stochastic model of each disease.
- Each disease has three successive stages.
- We know the daily probability of each state transition.
- We know the probability of each temperature at each stage.

Which is more likely, disease A or disease B?

Example: The Model



Direct Simulation is Problematic

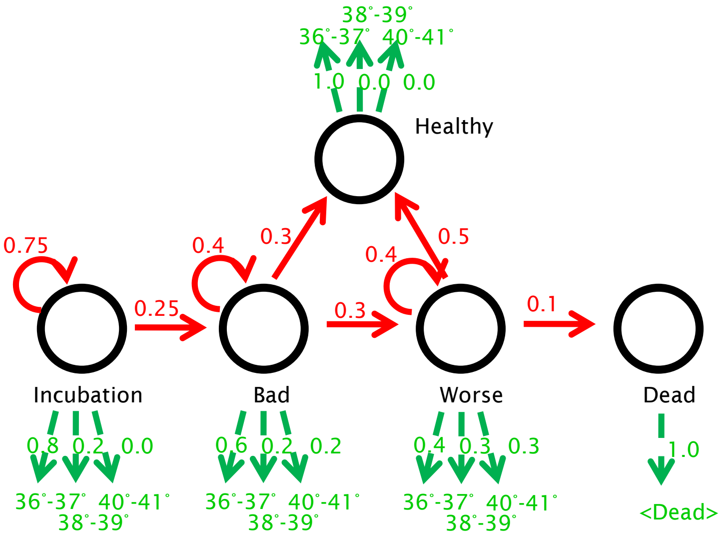
This model will allow us to perform a simulation.

What can the simulation show us?

- Individual samples of the dynamics of an unspecified patient.

But what if we have a specific patient with specific symptoms?

- We would have to perform replications until we have seen the trace a sufficient number of times.
- This could take a very long time!



Hidden Markov Chains

A Hidden Markov Chain …

- is based on a Markov chain,
- permits symbols to be emitted in each state,
- associates probabilities with each symbol emission.

A *trace* is given:

- A sequence of symbols that has been emitted by the HMM

Questions that can be answered for a given HMM:

- What is the probability that it will produce the trace?
- What is the probability that a certain sequence of state changes generates the trace?

Applications

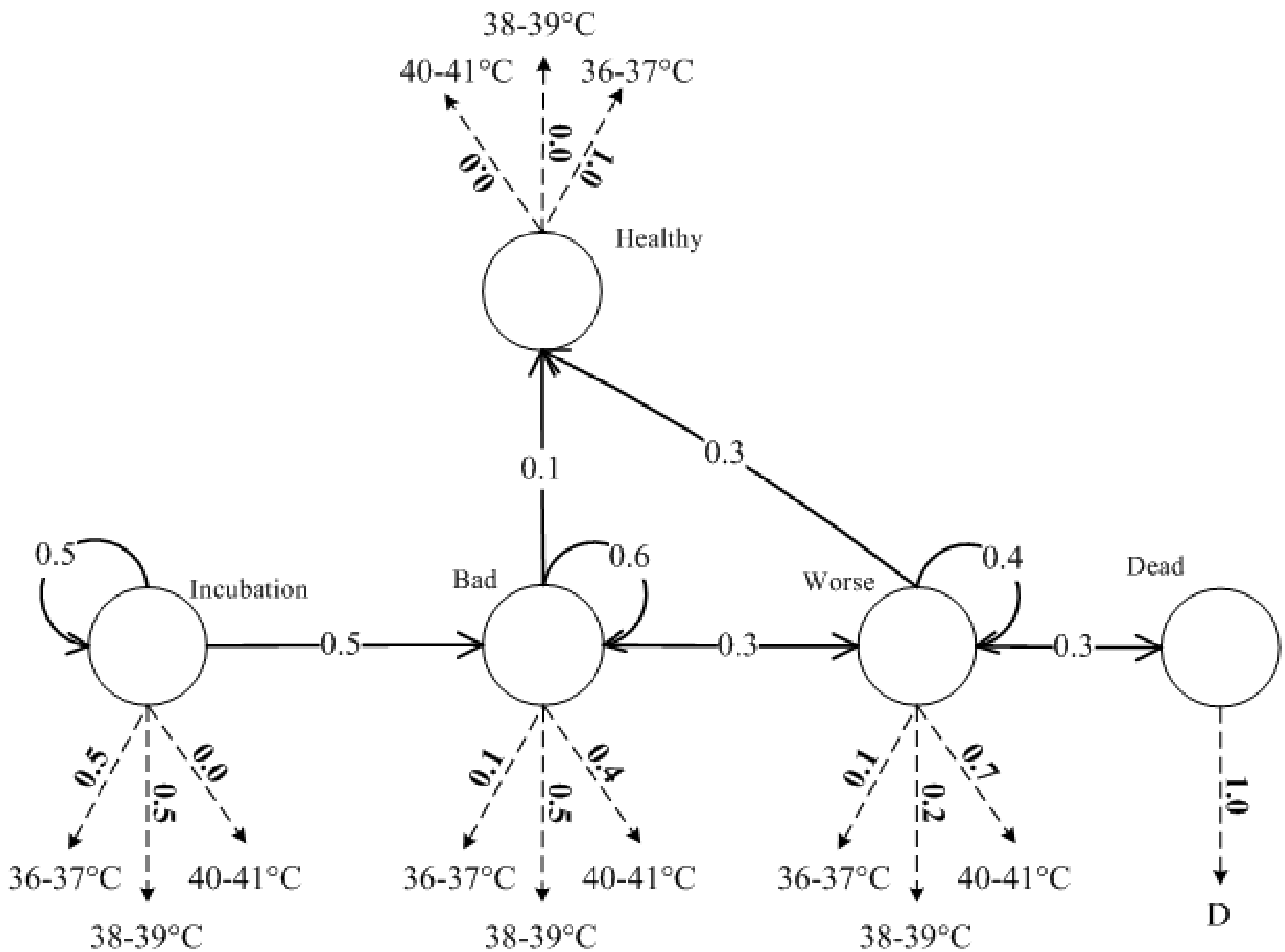
When are HMMs used?

- To recover unobservable data sequences that can be inferred from associated data.

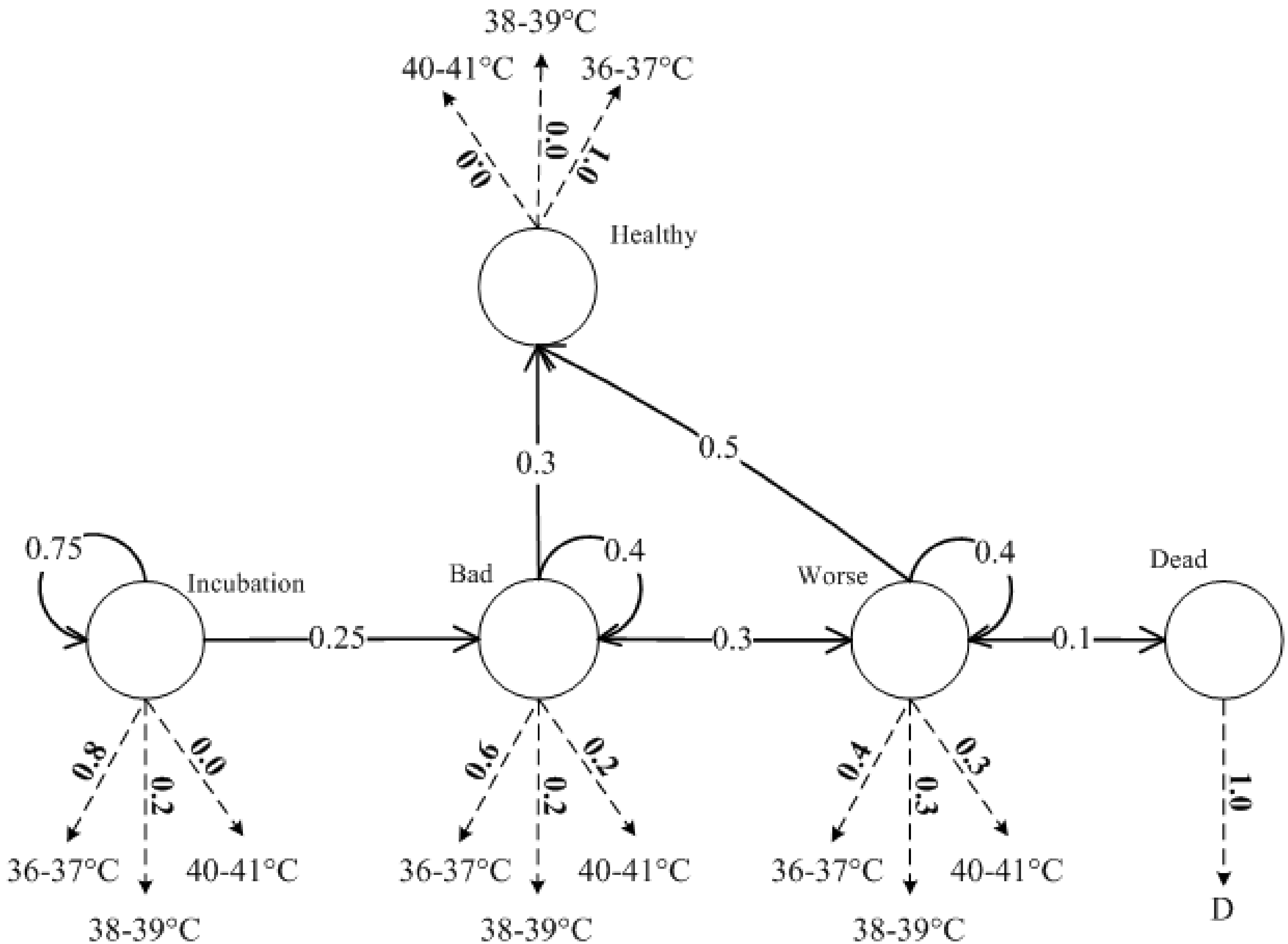
Some examples:

- Handwriting recognition
- Speech recognition
- Gesture recognition
- Bioinformatics
- Cryptoanalysis

Model of Disease A



Model of Disease B



Nomenclature

We have a set of states S:

$$S = \{Incubate, Bad, Worse, Healthy, Dead\}$$

We have a set of output symbols V:

$$V = \{36/37,\ 38/39,\ 40/41,\ Dead\}$$

We have the probabilities for the initial state:

$$\Pi = (1,\ 0,\ 0,\ 0,\ 0)$$

The Analysis Task

Given a sequence of observations O, …

- For example, …

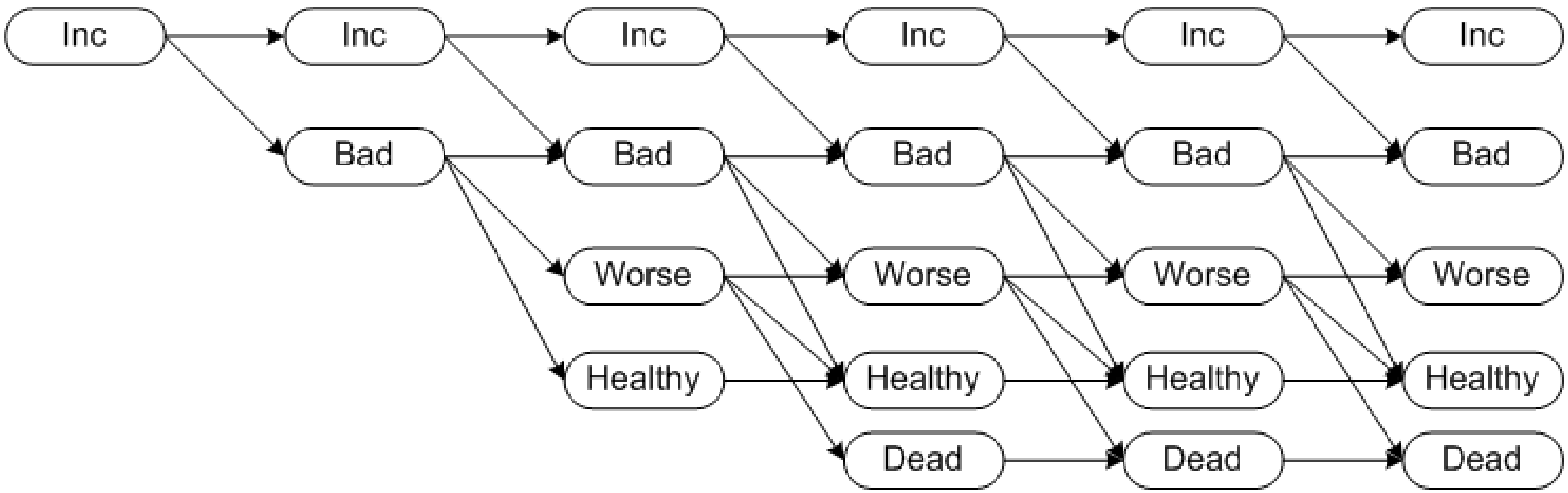
$$O = (36,\ 37,\ 37,\ 40,\ 39,\ 37)$$

The task:

- Compute which disease is more probable.

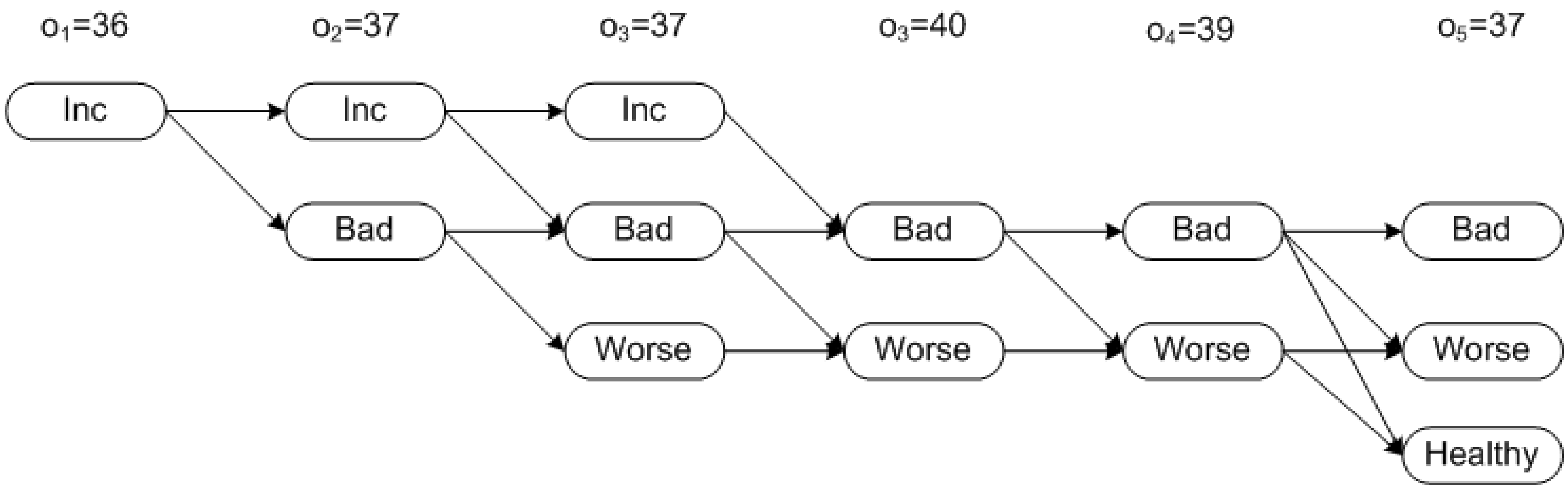
Analysis

The set of all possible paths of length 6:



Analysis

The set of all paths that are consistent with the observation O:



Solution for Disease A

Compute the probability that model A will produce the trace.

Table of results:

Symbol	Incubate	Bad	Worse	Healthy	Dead
	1,000000	0,000000	0,000000	0,000000	0,000000
36°	0,500000	0,000000	0,000000	0,000000	0,000000
37°	0,125000	0,025000	0,000000	0,000000	0,000000
37°	0,031250	0,007750	0,000750	0,002500	0,000000
40°	0,000000	0,008110	0,001838	0,000000	0,000000
39°	0,000000	0,002433	0,000634	0,000000	0,000000
37°	0,000000	0,000146	0,000098	0,000433	0,000000

Total probability of the last row $= 0.000678$

Solution for Disease B

The analogous table for disease B:

Symbol	Incubate	Bad	Worse	Healthy	Dead
	1,000000	0,000000	0,000000	0,000000	0,000000
36°	0,800000	0,000000	0,000000	0,000000	0,000000
37°	0,480000	0,120000	0,000000	0,000000	0,000000
37°	0,288000	0,100800	0,014400	0,036000	0,000000
40°	0,000000	0,022464	0,010800	0,000000	0,000000
39°	0,000000	0,001797	0,003318	0,000000	0,000000
37°	0,000000	0,000431	0,000746	0,002198	0,000000

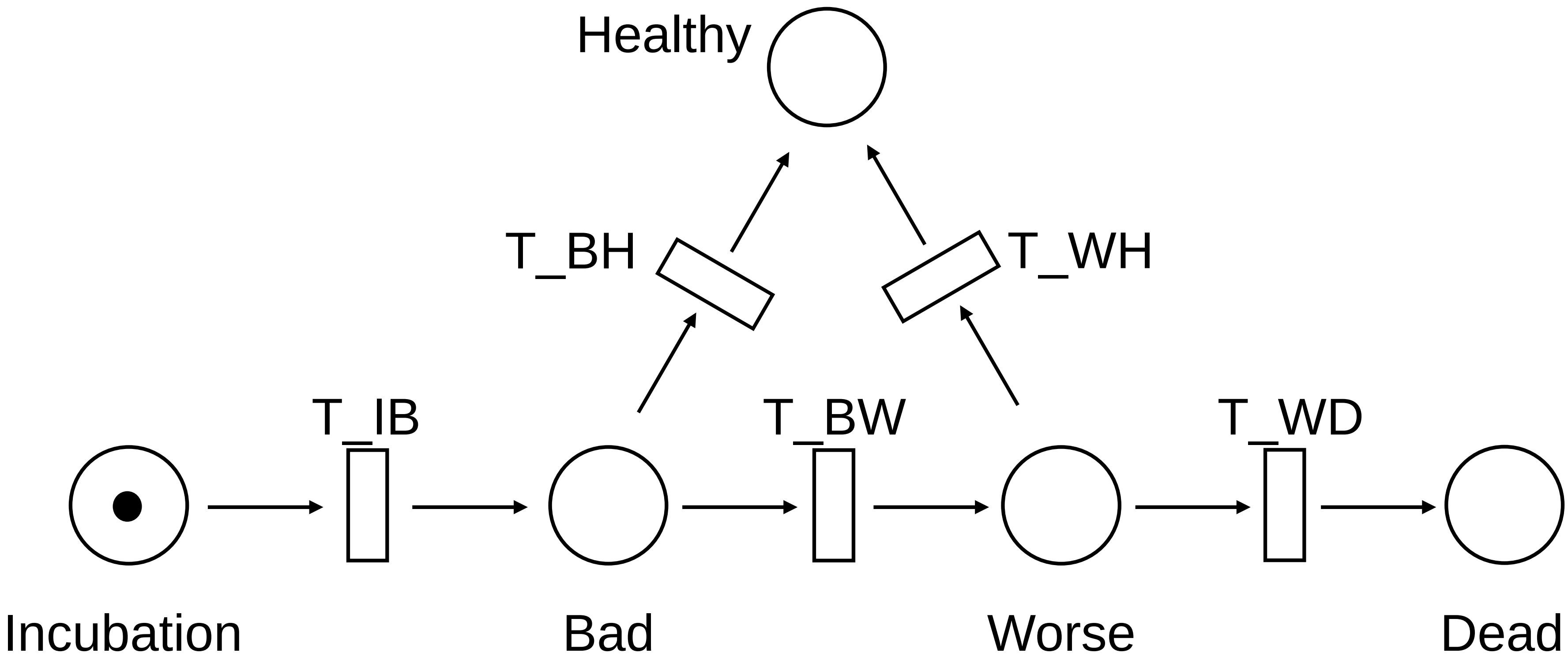
Total probability of the last row $= 0.003376$

→ Disease B is more likely!

A Real Time Model

Consider now a real-time model.

- The state changes may have rates with general distributions.



A Real Time Model

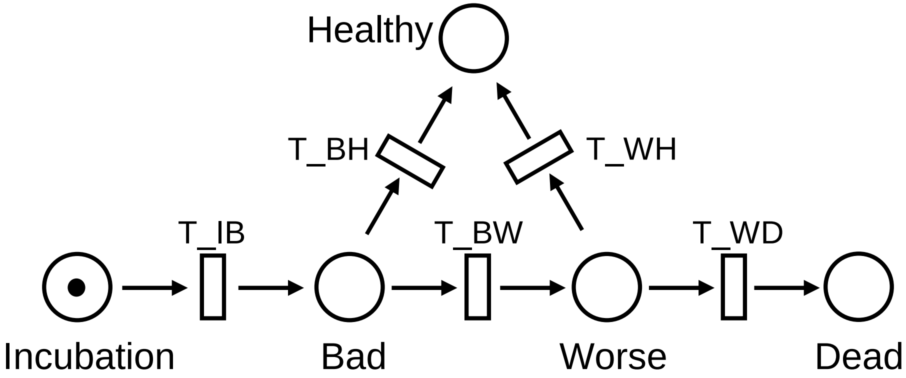
Important consequence:

- The model no longer corresponds to a Markov chain.

Why not?

- The state transition probabilities change as time progresses.

Until now, this case could not be modelled and simulated.



Research at the LfS

Research at the LfS is concerned with hidden models.

We are interested in a more general case.

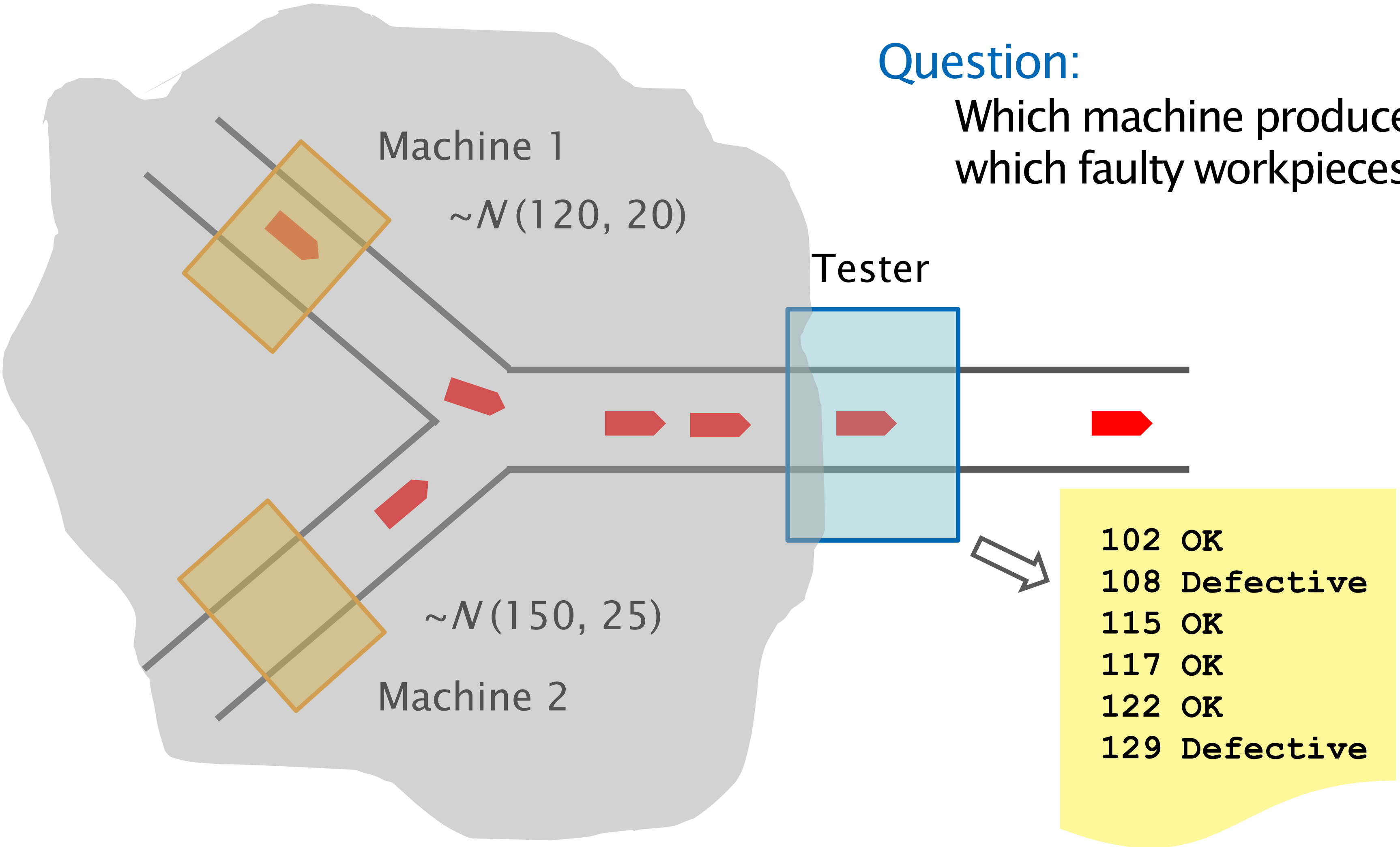
- The stochastic process is not a Markov chain.

Some results:

- The HMM functionality can be achieved.
- However, many extra states must be added.
- The underlying Markov chain becomes larger and more complex.
- Several interesting possibilities are opened up.

→ Master-Module *Applied Discrete Modelling*

An Industrial Application



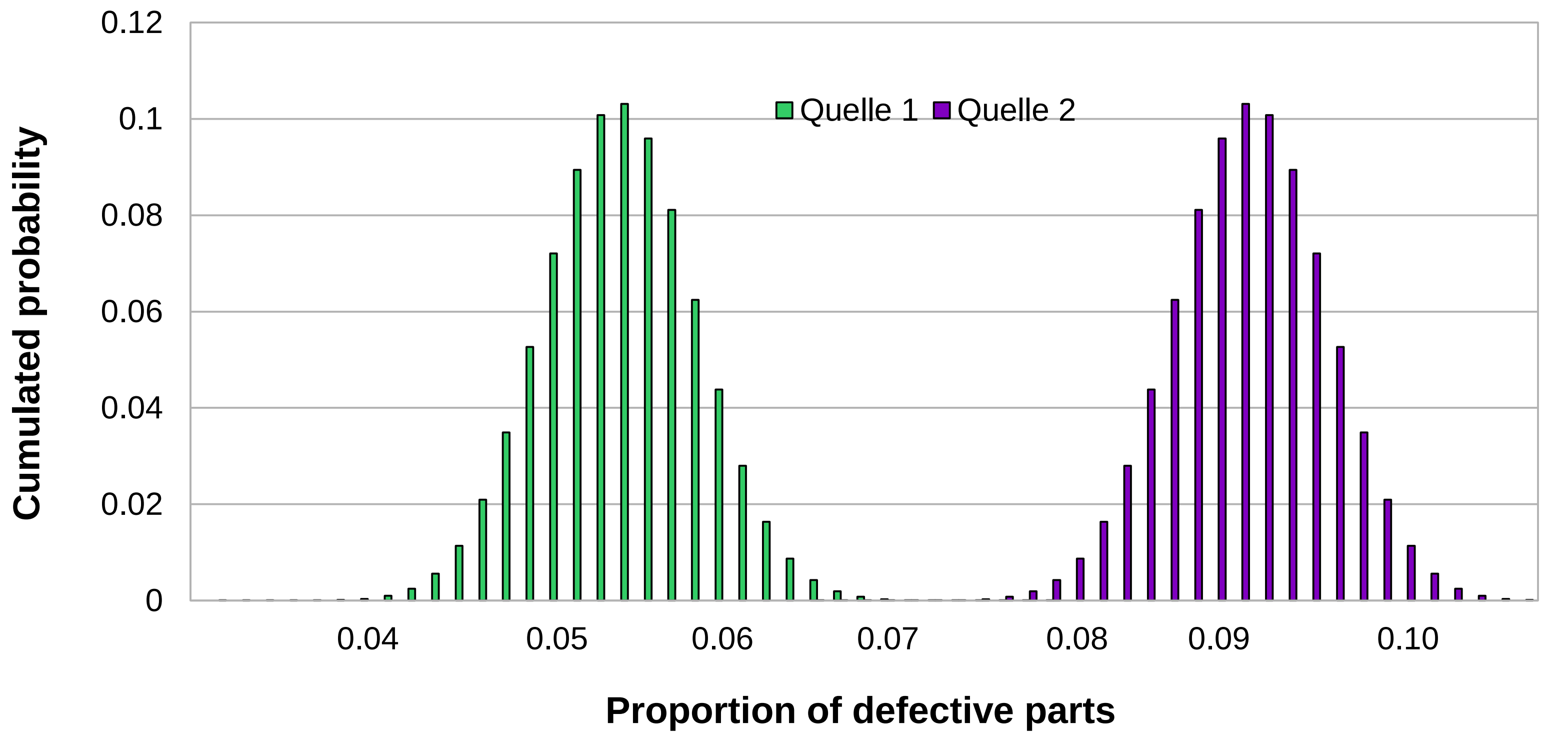
Question:

Which machine produces which faulty workpieces?

A Simulation Result

Distribution of the error probabilities for each machine

- Machine 2 causes about twice as many errors as Machine 1.



Virtual Sensors

A *virtual sensor* is …

- A sensor that measures one quantity in order to infer a different one.

Example:

- Use the electrical measurements of a sparking plug to determine the properties of the fuel mix.

Virtual sensors have existed for a long time.

- They are used for continuous, physical, deterministic variables.

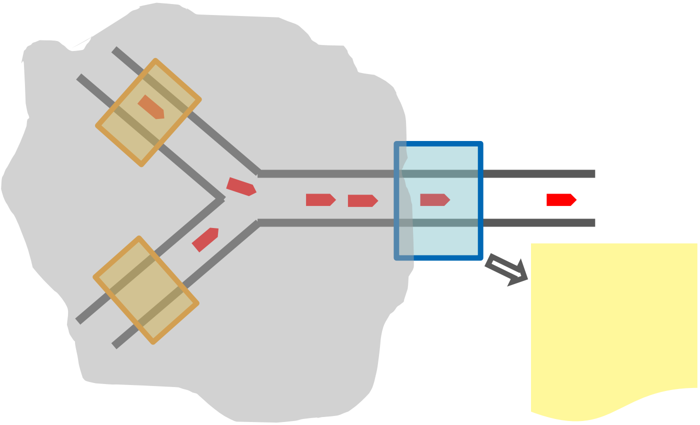
Virtual Stochastic Sensors

A virtual stochastic sensor is …

- A sensor that measures one stochastic quantity in order to infer a different one.

Example:

- Use the tester results in order to "virtually observe" the machines' behaviour.



Virtual stochastic sensors are an invention of the LfS.

Current Research

Some of our current research questions

- What configurations are possible for virtual stochastic sensors?
- How do accuracy and computation time depend on the specific configuration?
- Can we develop efficient algorithms for specific classes of model?
- How much information must a symbol sequence have in order to reveal hidden system behaviour?

Scientific Papers

Robert Buchholz, Claudia Krull, Thomas Strigl, Graham Horton:

- Using Hidden non-Markovian Models to Reconstruct System Behaviour in Partially-Observable Systems

Claudia Krull, Graham Horton:

- Hidden Non-Markovian Models: Formalization and Solution Approaches

Claudia Krull, Robert Buchholz, Graham Horton:

- Matching Hidden Non-Markovian Models: Diagnosing Illnesses Based on Recorded Symptoms

To be found at http://www.sim-md.de → Forschung

Learning Goals

Questions to test your knowledge:

- How is a DTMC defined?
- What is the mathematical representation of a DTMC?
- How would you compute the solution of a DTMC?
- Sketch the DTMC that is described by the following scenario: …
- What is a Hidden Markov Chain? What is it used for?