Mathematical Modelling FK (FRTN45)
F2

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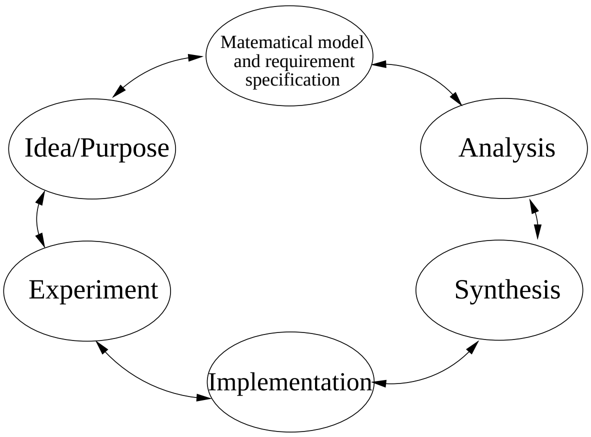
Modelling in three phases:

1. Problem structure
   - **Formulate purpose**, requirements for accuracy
   - Break up into subsystems — What is important?
2. Basic equations
   - Write down the relevant physical laws
   - Collect experimental data
   - Test hypotheses
   - Validate the model against fresh data
3. Model with desired features is formed
   - Put the model on suitable form. (Computer simulation or pedagogical insight?)
   - Document and illustrate the model
   - Evaluate the model: **Does it meet its purpose?**



Outline

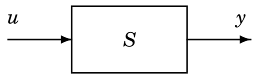
Thursday lecture

- Course introduction
- Ethics of modelling
- Static models from data (black boxes)

Friday lecture

- **Dynamic models from data (black boxes)**
- Models from physics (white boxes)
- Mixed models (grey boxes)

Basic idea of system identification



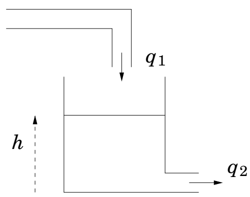
Measure U and y. Figure out a model of S, consistent with measured data.

Important aspects:

- We can only measure the u and y in discrete time points (sampling). Can be natural to use the discrete-time models.
- The system is affected by interference and measurement errors. We may need to signal models for dealing with this.

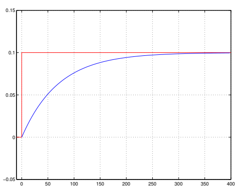
Example

A tank which attenuates flow variations in q_1. Characterization of the tank system:



- Input: q_1
- Output: q_2 and/or h
- Internal variables / conditions: h

Step response

Step response for the tank 

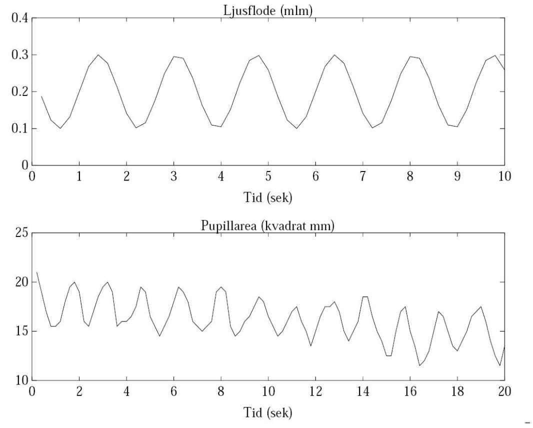
Can give idea of the dominant time constant, static reinforcement, character (overshoot or not)

Frequency response

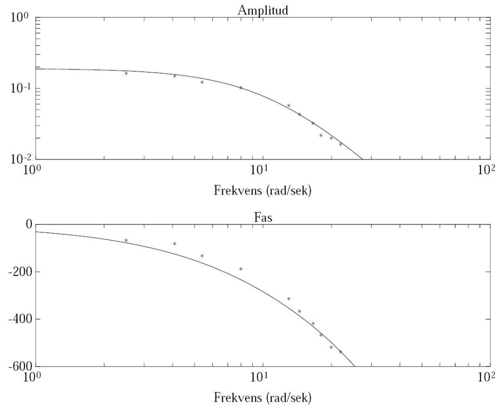
For good signal-to-noise ratio, an estimate of $G(i\omega)$ is obtained directly from the amplitudes and phase positions of u, y

$$\begin{aligned} u(t) &= A \sin \omega t \\ y(t) &= A|G(i\omega)| \sin(\omega t + \arg G(i\omega)) \end{aligned}$$

How light affects pupil area



Bode-diagram for pupil



Correlation analysis

Can we estimate the impulse response with other inputs?

- Impulse response formula in discrete time ($T = 1$, $v =$ noise):

$$y(t) = \sum_{k=1}^{\infty} g_k u(t-k) + v(t)$$

- If v white noise with $\mathbf{E}v^2 = 1$, then

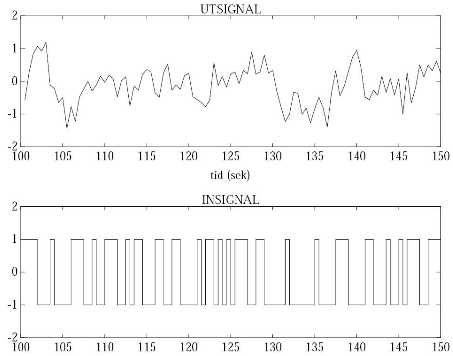
$$R_{yu}(k) = \mathbf{E}y(t)u(t-k) = g_k$$

- Covariance R_{yu} estimated by N data points with

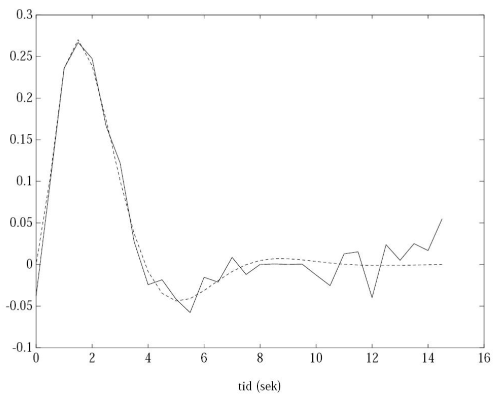
$$\widehat{R}_{yu}^N(k) = \frac{1}{N}\sum_{t=1}^{N} y(t)u(t-k)$$

Example

Correlation analysis for $\frac{1}{s^2+2s+1}$ (in- and out-put data)



Estimated and actual impulse responses



Basic rules

Make experiments with conditions similar to the conditions in which the model is to be used!

(Models from step response can be expected to work best on the stage.)

Save some data for model validation, i.e. check the model with data set different from the one that generated the model!

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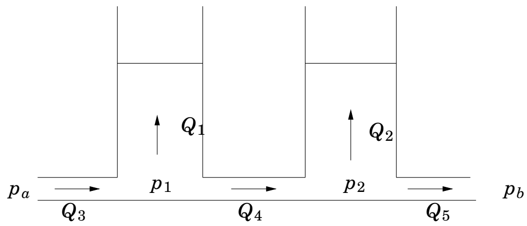
Principles and analogies: Hydraulics

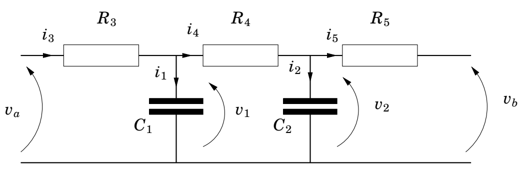
Example 1. A hydraulic system:



Incompressible fluid. Pressures: p_a, p_1, p_2, and p_3.
Volume flows: Q_1, Q_2, Q_3, Q_4, and Q_5.

Principles and analogies: Electrics

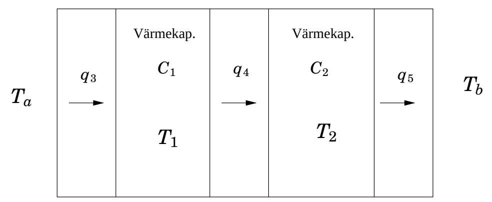
Example 2. An electrical system:



Potentials v_a , v_b , v_1, and v_2
Currents i_1 , i_2, i_3, i_4, and i_5

Principles and analogies: Heat

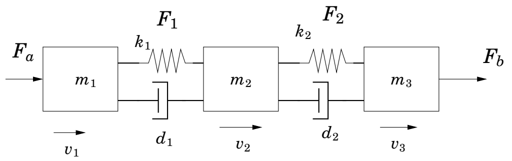
Example 3. A thermal system
(heat transfer through a wall):



Two elements with thermal capacities C_1 and C_2 separated by insulating layers. Heat flows: q_3 , q_4 and q_4
Temperatures: T_a , T_b , T_1 and T_2

Principles and analogies: Mechanics

Exempel 4. A mechanical system:



External forces: F_a and F_b
Velocities: v_1, v_2 and v_3
Spring constants: k_1 and k_2
Damping constants: d_1 and d_2

Analogies

Analogies: hydraulic - electric - thermal - mechanical
Two types of variables:

A. Flow Variables
- volume flow
- power flow
- heat flow
- speed

B. Intensity variables
- pressure
- voltage
- temperature
- force

For both of them addition rules hold.

Analogies (cont'd)

Intensity variations

$$C \cdot \frac{d}{dt}(\text{intensity}) = \text{flow}$$

C "capacitance":
hydraulic: $A/(\rho g)$
electrical: kapacitans
heat: thermal capacity
mechanical: inverse spring constant
Balance equations!

(More complicated if the capacitance is not constant.)

Analogies (cont'd)

Losses

$$\text{flow} = \phi(\text{intensity})$$

$$\text{intensity} = \varphi(\text{flow})$$

Hydraulic: flow resistance
Electrics: resistance
Heat: thermal conductivity
Mechanics: friction

Often linear relationship in the electrical case - nonlinearly in the other (may be approximated by linear for small changes of variables)

More phenomena

Intensity variations

$$L \cdot \frac{d}{dt}(\text{flow}) = \text{intensity}$$

L "inductance"
hydraucs: $\rho l/A$
electrics: inductans
heat: –
mechanics: mass
balance equations!

(more complicated if the inductance is not constant.)

Energy flows

Can you make a general modeling theory based on flow and intensity variables? Note the following.

$$\begin{aligned}
\text{pressure} \cdot \text{flow} &= \text{power}\\
\text{voltage difference} \cdot \text{current} &= \text{power}\\
\text{force} \cdot \text{velocity} &= \text{power}\\
\text{torque} \cdot \text{angular velocity} &= \text{power}\\
\text{temperature} \cdot \text{heat flow} &= \text{power} \cdot \text{temperature}
\end{aligned}$$

Dimension analysis

Physical variables have dimensions. E.g.,

$$[\text{density}] = ML^{-3}$$
$$[\text{force}] = M \cdot \frac{L}{T^2} = MLT^{-2}$$

where

$$M = [\text{mass}], \quad T = [\text{time}], \quad L = [\text{length}]$$

Physical connections must be dimensionally “correct”.

Example: Bernoulli’s law

In Bernoulli’s law $v = \sqrt{2gh}$ you have

$$[v/\sqrt{gh}] = LT^{-1}(LT^{-2}L)^{-0.5} = 1$$

$v/\sqrt{gh}$ is an example of dimensionless quantity.

Dimensionless quantities and scaling

Some historical passanger ships:

- Kaiser Wilhelm the great, 1898, 22 knots, 200 m
- Lusitania, 1909, 25 knots, 240 m
- Rex, 1933, 27 knots, 269 m
- Queen Mary, 1938, 29 knots, 311 m

Note that the ratio *(velocity)*^{2}*/(length)* is almost constant

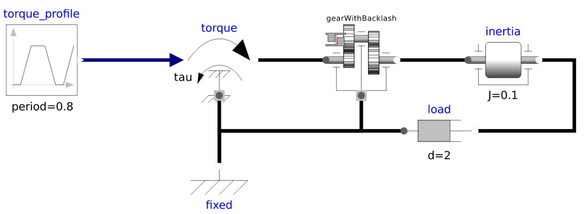
Which physical phenomenon can be thought to be the cause?

2 min problem

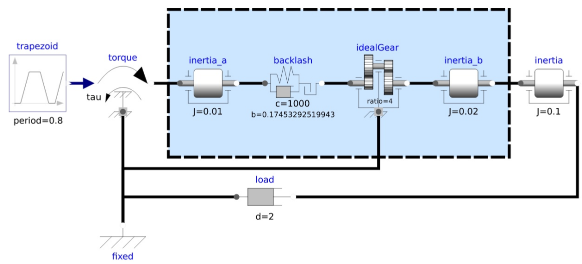
Find the relationship (except for a scaling by a dimensionless constant) between a pendulum period time and its mass, its length and the acceleration of gravity g, i.e.,

$$t = f(m, l, g)$$

A Graphical Modelica Model



A submodel can be opened



Simple system in text format

```
model FirstOrder
  Real x;
equation
  der(x) = 1-x;
end FirstOrder;
```

Documentation is important:

```
model FirstOrderDocumented "A simple first order differential equation"
  Real x "State variable";
equation
  der(x) = 1-x "Drives value of x toward 1.0";
end FirstOrderDocumented;
```

Initialize at equilibrium!

```
model FirstOrderSteady
  "First order equation with steady state initial condition"
  Real x "State variable";
initial equation
  der(x) = 0 "Initialize the system in steady state";
equation
  der(x) = 1-x "Drives value of x toward 1.0";
end FirstOrderSteady;
```

A predator-prey model

$$\begin{cases} \dot{x} = x(\alpha - \beta y) \\ \dot{y} = y(\delta x - \gamma) \end{cases}$$

```
model ClassicModel "This is the typical equation-oriented model"
  parameter Real alpha=0.1 "Reproduction rate of prey";
  parameter Real beta=0.02 "Mortality rate of predator per prey";
  parameter Real gamma=0.4 "Mortality rate of predator";
  parameter Real delta=0.02 "Reproduction rate of predator per prey";
  parameter Real x0=10 "Start value of prey population";
  parameter Real y0=10 "Start value of predator population";
  Real x(start=x0) "Prey population";
  Real y(start=y0) "Predator population";
equation
  der(x) = x*(alpha-beta*y);
  der(y) = y*(delta*x-gamma);
end ClassicModel;
```

Re-using old models

Inheritance:

```
model QuiescentModelWithInheritance "Steady state model with inheritance"
  extends ClassicModel;
initial equation
  der(x) = 0;
  der(y) = 0;
end QuiescentModelWithInheritance;
```

Modfication:

```
model QuiescentModelWithModifications "Steady state model with modifications"
  extends QuiescentModelWithInheritance(gamma=0.3, delta=0.01);
end QuiescentModelWithModifications;
```

Nonlinear differential-algebraic equations (DAE)

Differential-algebraic equations, DAE

$$F(\dot{z}, z, u) = 0, \quad y = H(z, u)$$

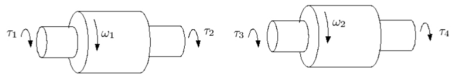
u: input, y: output, z: "internal variable"

Special case: state model

$$\dot{x} = f(x, u), \quad y = h(x, u)$$

u: input, y: output, x: state

Mathematics of general connection:



State models for two separate components:

$$\begin{aligned} \dot{\phi}_1 &= \omega_1 \\ J_1\dot{\omega}_1 &= \tau_1 + \tau_2 \end{aligned} \qquad \begin{aligned} \dot{\phi}_2 &= \omega_2 \\ J_2\dot{\omega}_2 &= \tau_3 + \tau_4 \end{aligned}$$

Connection:

$$\begin{aligned} \phi_1 &= \phi_2 \\ \tau_2 &= -\tau_3 \end{aligned}$$

The resulting model is not exactly a state model.

Linear differential-algebraic equations (DAE)

$$E\dot{z} = Fz + Gu$$

If E were non-singular, one could write

$$\dot{z} = E^{-1}Fz + E^{-1}Gu$$

which is a valid state model. If E is singular, variables have to be eliminated to get a state equation. Using a DAE solver is often better, since elimination can destroy sparsity.

Example:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & J_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & J_2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{\phi}_1 \\ \dot{\omega}_1 \\ \dot{\phi}_2 \\ \dot{\omega}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \omega_1 \\ \phi_2 \\ \omega_2 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \end{bmatrix}$$

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Prediction Error Methods

Find the unknown parameters θ by optimization:

$$\min_{\theta} \|\hat{y}(t, \theta) - y(t)\|$$

Here $y(t)$ is the measured output at time t and $\hat{y}(t, \theta)$ is the predicted output based on past measurements using a model with parameter values θ.

Prediction Error Method with Repeated Simulation

For a nonlinear grey-box model

$$\begin{aligned} 0 &= F(\dot{x}, x, t, \theta) \\ y(t) &= h(x, t, \theta) \end{aligned}$$

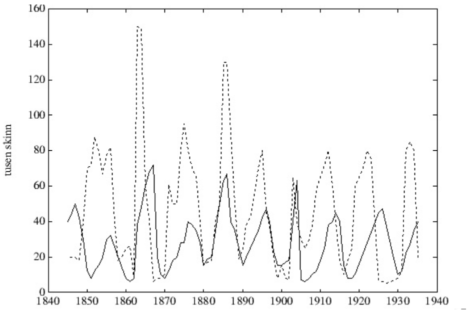
the unknown parameters θ could be determined by the prediction error method

$$\min_{\theta} \|\hat{y}(t, \theta) - y(t)\|$$

where the output prediction $\hat{y}(t, \theta)$ is computed by simulation.

(Repeated simulation for different values of θ could however be very time-consuming.)

Population dynamics / Ecology



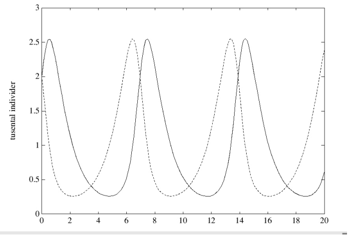
Variations in the number of lynx (solid) and hares (dashed) in Canada. Can you predict the periodic variations?

Population dynamics

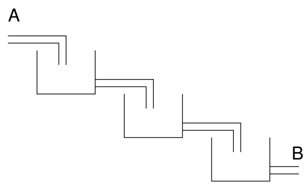
N_1 number of lynx, N_2 number of hares

$$\frac{d}{dt}N_1(t) = (\lambda_1 - \gamma_1)N_1(t) + \alpha_1 N_1(t)N_2(t)$$
$$\frac{d}{dt}N_2(t) = (\lambda_2 - \gamma_2)N_1(t) - \alpha_2 N_1(t)N_2(t)$$

Simulation:



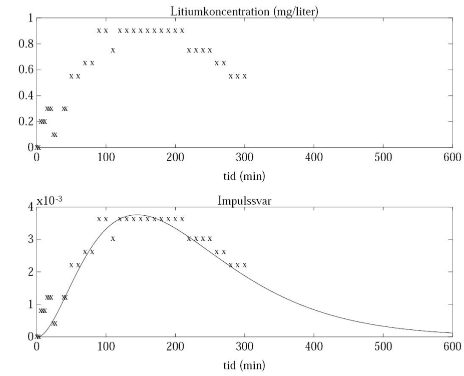
Mixing tanks in Skärblacka paper factory



A linear transfer function of three series-connected mixing tanks has the form $\frac{1}{(s\theta+1)^3}$.

To determine θ, radioactive lithium is added in **A**. Radioactivity was then measured by **B** as a function of time.

Impulse response

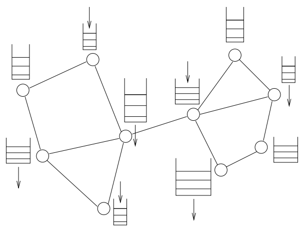


In the lower picture, θ has been chosen to adapt to the impulse response of $\frac{1}{(s\theta+1)^3}$

Grey Models — the best of both worlds

- White boxes: Physical laws provide some insight
- Black boxes: Statistics estimates complex relationships
- Gray boxes: Combine simplicity with insight

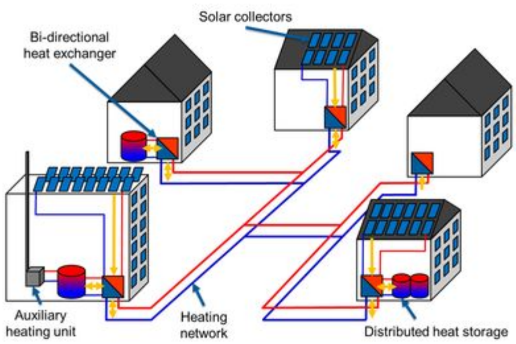
My Own Research: Dynamic Buffer Networks



- Producers, consumers and storages
- Examples: water, power, traffic, data
- Discrete/continuous, stochastic/deterministic
- Multiple commodities, human interaction

Problem: Scalable and adaptive methods for control.

Example: Heating Networks



Grey box modelling!

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Good luck with your projects!

I look forward to receiving your project plans.