Introduction to Research

Arun K. Tangirala

Modelling Skills

Objectives

To learn the following:

- What is a model?
- First-principles (mechanistic) vs. empirical models.
- Systematic procedure for building models from data.
- Few critical aspects of data-driven (empirical) modelling.

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- Systematic procedure for building models from data.
- Few critical aspects of data-driven (empirical) modelling.

With two hands-on examples in R® (a popular software for data analysis) . . .

What is a model?

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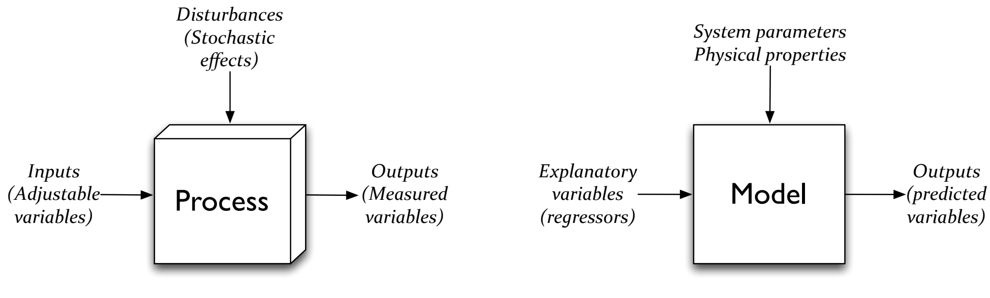
For the purposes of

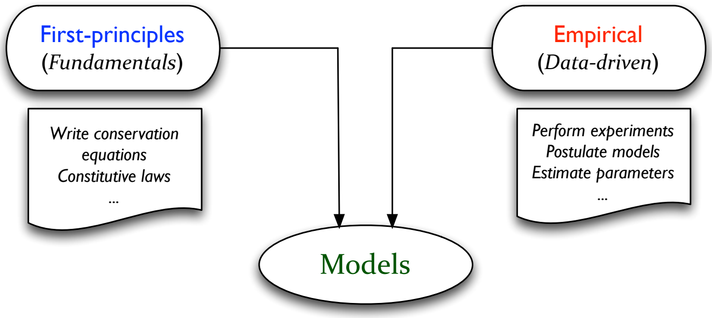
- Prediction (inferring the unknowns)
- Classification (pattern recognition)
- Fault detection
- Process simulation
- Design and optimization
- ...

Model vs. process



A model emulates the process given the operating conditions, parameters and physical properties. However, in general, its architecture is different from the process!

Two broad approaches to modelling



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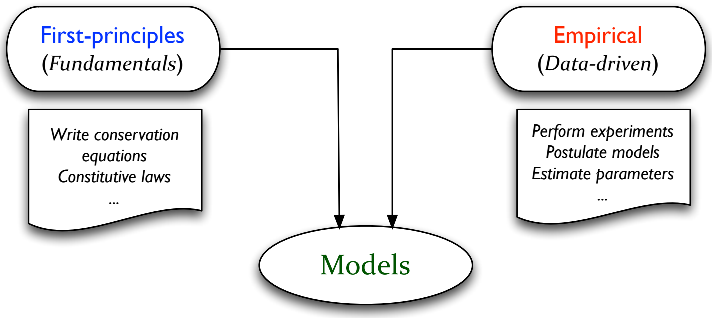


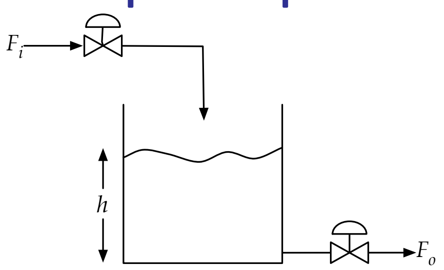
Test drive of a vehicle

Taking a vehicle for a test drive is a simple example of how experiments are a natural way of understanding processes. As the vehicle is subjected to different test (road) conditions, its response is used by the test-driver to develop a "mental model" of the vehicle.

First-principles vs. Empirical modelling

First-principles	Empirical
Causal, continuous, non-linear differential-algebraic equations	Models are usually black-box and discrete-time
Model structures are quite rigid - the structure is decided by the equations describing fundamental laws.	Model structures are extremely flexible - implies they have to be assumed/known a priori.
Can be quite challenging and time-consuming to develop	Relatively much easier and are less time-consuming to develop
Require good numerical ODE and algebraic solvers.	Require good estimators (plenty of them available)
Very effective and reliable models - can be used for wide range of operating conditions	Model quality is strongly dependent on data quality - usually have poor extrapolation capabilities
Transparent and can be easily related to physical parameters/characteristics of the process	Difficult to relate to physical parameters of the process (black-box) and the underlying phenomena

Example: Liquid level system



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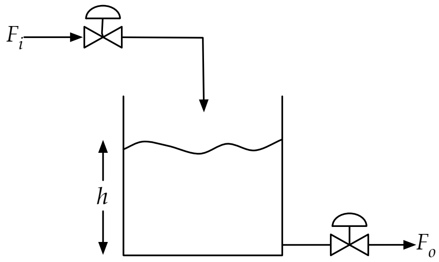

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$$F_o = C_v \sqrt{h}$$

(C_v is estimated from data)

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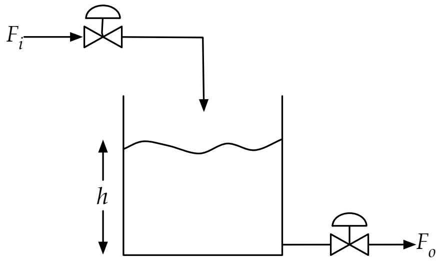

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Case 2: **Dynamic, non-linear** model of $h(t)$ for changes in $F_i(t)$.

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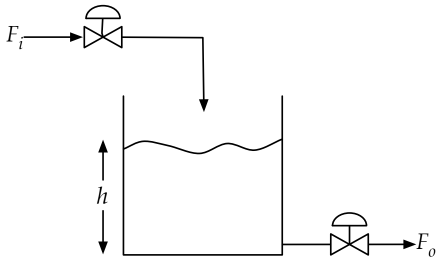

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Case 3: **Approximate linear, dynamic** model about an operating point

$$A_c\frac{d\tilde{h}}{dt} = \tilde{F}_i - \beta\tilde{h}, \quad \beta = \frac{C_v}{2\sqrt{h_s}}$$
$$\tilde{F}_i = F_i - F_s, \tilde{h}_i = h_i - h_s$$

Typically, h_s, F_s are steady-state values.

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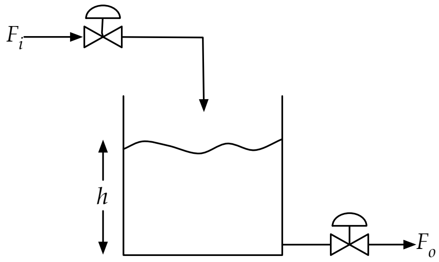

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Case 4: Approximate **empirical, linear**, **grey-box**, **dynamic, discrete-time** model,

$$h[k] = a_1 h[k-1] + b_i F_i[k-1] + \varepsilon[k]$$

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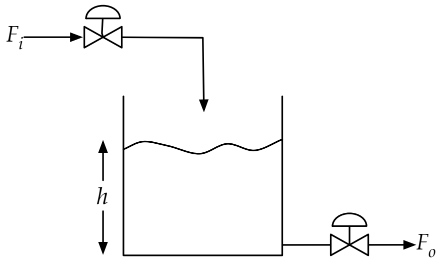

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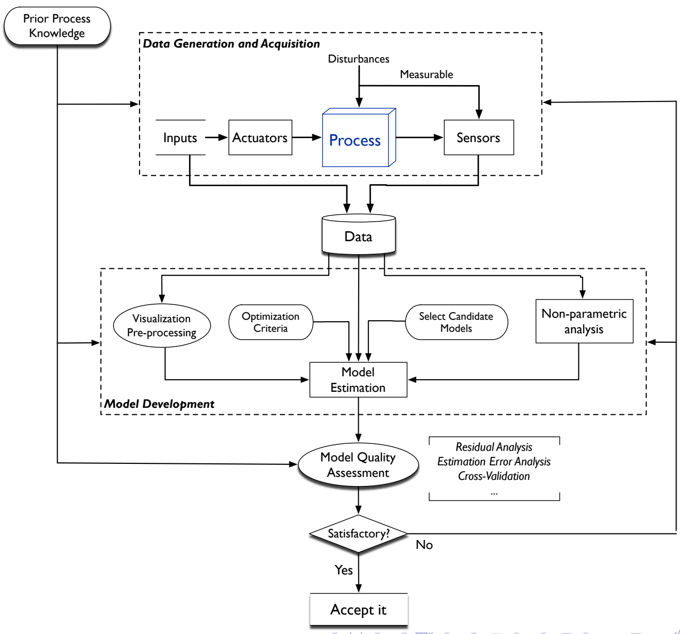
Case 5: **Black-box, dynamic, discrete-time model**

1. Model structure based on ease of estimation and end-use
2. Model may not be physically interpretable, but designed to give good predictions.

Building models from data: systematic procedure

- Primarily one finds three stages, which again contain sub-stages
- All models should be subjected to a critical validation test
- Final model quality largely depends on the quality of data
- Generating rich (informative) data is therefore essential



Two broad classes of models

Time-series models

- Suited for modelling stochastic or random processes (e.g., stock market index, rainfall, sensor noise)
- Causes are either unknown or also random
- Usually dynamic models (in a few applications, steady-state as well)
- Challenges: choosing model structure, making the right assumptions on process characteristics, non-linearities, etc.

Two broad classes of models ...contd.

Input-output or causal models

- Suited for modelling relationship between a variable (or more) and other **explanatory** variables (a.k.a. **regressors** or **factors**) (e.g., power and current in a wire, temperature and coolant flow)
- Regressors may be known accurately or with some error
- Models could be steady-state or dynamic.
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Remember

In practice, all modelling exercises demand a careful handling of uncertainties both at the experimental and modelling stages!

Excite the process sufficiently!

Example

Consider a steady-state model:

$$y[k] = b_0 + b_1 u[k] + b_2 u^2[k]$$

- Three unknowns
- Therefore, data corresponding to three steady-states is required
- A more general statement: The regressor matrix

$$\mathbf{U} = \begin{bmatrix} 1 & u[k_1] & u^2[k_1] \\ 1 & u[k_2] & u^2[k_2] \\ 1 & u[k_3] & u^2[k_3] \end{bmatrix} \tag{1}$$

should be non-singular, i.e., of full rank.

For dynamic systems

Example

Consider a (deterministic) process:

$$y[k] = b_1 u[k-1] + b_2 u[k-2] + b_3 u[k-3]$$

Suppose that the process is excited with $u[k] = \sin(\omega_0 k)$ (sine of single frequency).

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$$\begin{aligned} y[k] &= b_1 \sin(\omega_0 k - \phi) + b_2 \sin(\omega_0 k - 2\phi) + b_3 \sin(\omega_0 - 3\phi) \\ &= \left(b_1 + \frac{b_2}{2\cos\omega_0}\right) \sin(\omega_0 k - \phi) + \left(b_3 + \frac{b_2}{2\cos\omega_0}\right) \sin(\omega_0 - 3\phi) \\ &= \left(b_1 + \frac{b_2}{2\cos\omega_0}\right) u[k-1] + \left(b_3 + \frac{b_2}{2\cos\omega_0}\right) u[k-3] \end{aligned}$$

Only two of the three parameters can be identified! Why?

Effects of randomness (noise) in data

The second challenging aspect of empirical modelling is the **presence of random or stochastic effects**.

Randomness (uncertainties) in the process influences identification in several ways:

- Accuracy of predictions
- Errors in parameter estimates
- Goodness of the deterministic model

Signal-to-Noise Ratio (SNR)

SNR

A key measure that quantifies the effects of noise is the **Signal-to-Noise Ratio** (SNR), which is defined as the ratio of variance of signal to the variance of noise in a measurement.

$$\text{SNR} = \frac{\sigma^2_{\text{signal}}}{\sigma^2_{\text{noise}}}$$

SNR can be interpreted as a measure of the degree of certainty (deterministic portion) to uncertainty

Example: Effect of SNR

Estimation of linear model from measured data

$$\textbf{Process} : x[k] = b_1 u[k-1] + b_0; b_1 = 5; b_0 = 2$$

Only $y[k] = x[k] + v[k]$ (measurement) is available. Goal is to estimate b_1, b_0.

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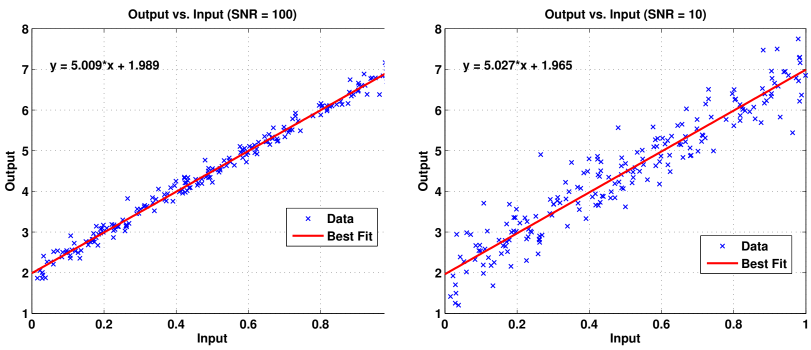

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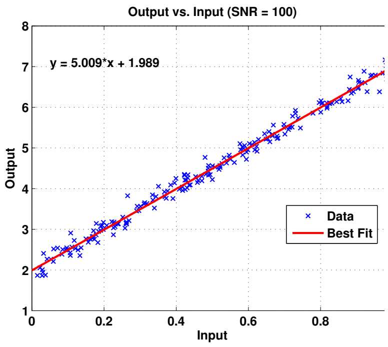

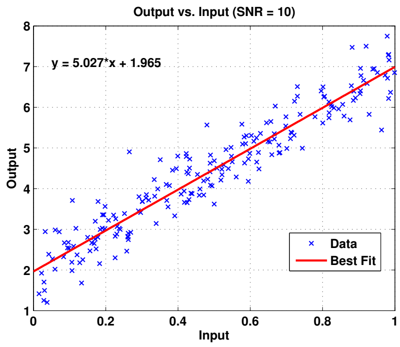

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Decrease in SNR increases the error in parameter estimates (proportional to $\sqrt{1/\text{SNR}}$)

Example: Overfitting

Process : $x[k] = 1.2 + 0.4u[k] + 0.3u^2[k] + 0.2u^3[k]$

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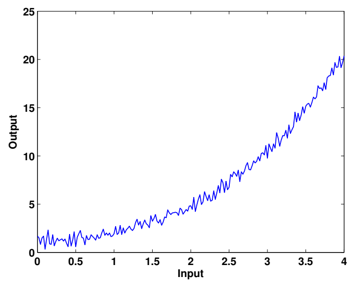

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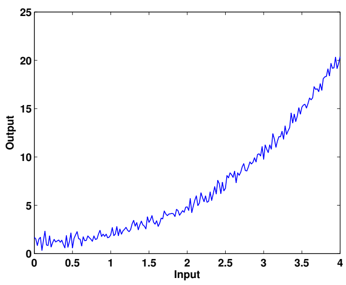

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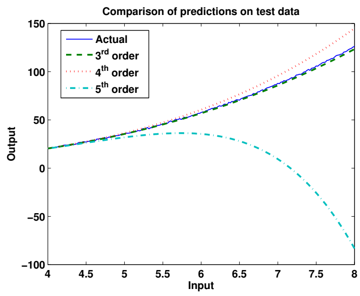

Cross-validation

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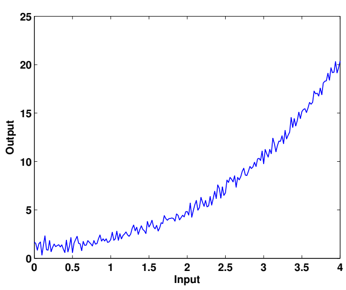

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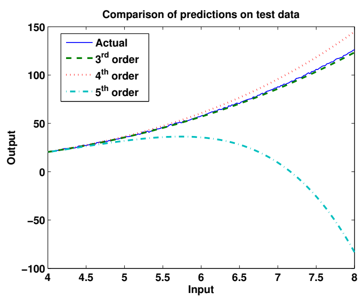

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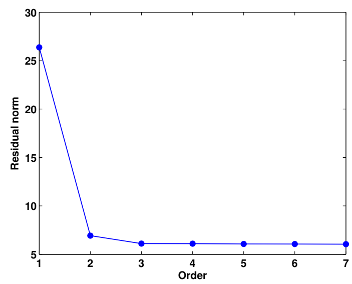

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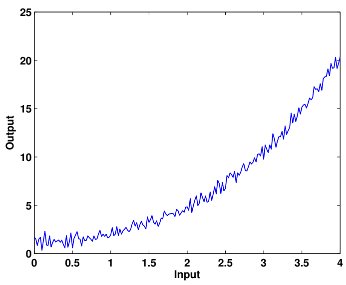

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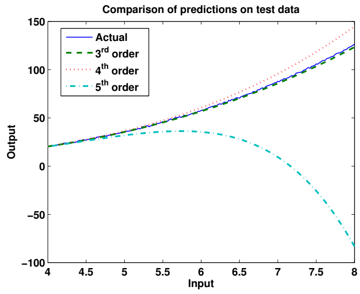

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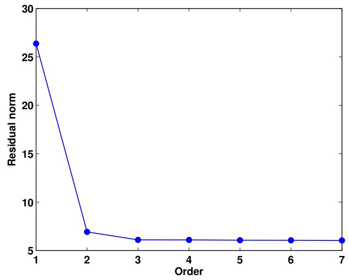

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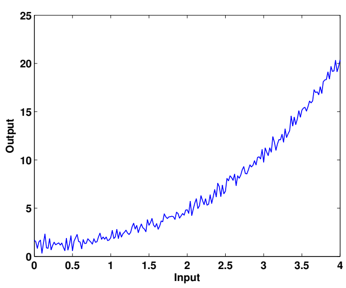

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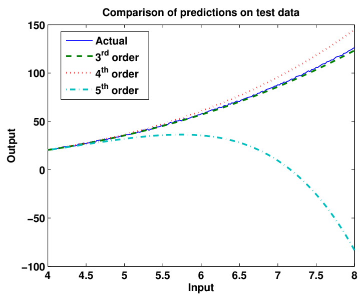

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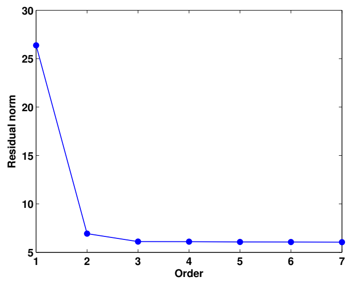

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3rd order fit: $\hat{y}[k] = \underset{(\pm 0.05)}{1.17} + \underset{(\pm 0.1)}{0.35}\, u[k] + \underset{(\pm 0.06)}{0.36}\, u^2[k] + \underset{(\pm 0.01)}{0.19}\, u^3[k]$

Questions for reflection

- What type of models are possible? Which one(s) to choose?
- How do we "fit" a model that "explains" the variations observed in experimental data?
- How to "correctly" account for the deterministic and stochastic effects?
- Will the experiment influence the model that we fit? If yes, in what way?
- How do we set up and solve the problem of estimating the unknown model parameters?
- What kind of experiments should we design to obtain a good quality model?
- How much data do we collect? (what should be the sample size?)

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