Fundaments of Machine learning for and with engineering applications

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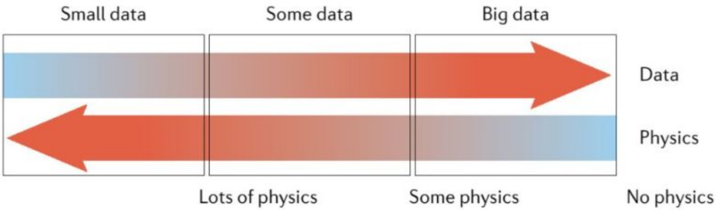
Sep 2, 2025

Data vs Physics



Uncertainty

- Def 1: Not knowing if an event is true or false. (Useful)
- Def 2: Things that cannot be measured. (Not useful)

Probability is how Uncertainty is quantified!

- Clarity test
- Assign a number between 0 and 1 to our degree of belief
- Error definition

Sentence also good for fortune cookies

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Random quotes

- Probability: there is not science more worthy in out contemplations nor a more useful one for admission to our system of public education
- The theory of probabilities is at the bottom of nothing but common sense reduced to calculus.

What is Statistics

Clarity test. Beer drinker?

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Data properties

1 D

logs

2 D: maps

Quite limited but great for visualization

3 D

3d maps, seismic cubes. More informative, mostly ok in digital formats.

4 D

Trajectories

x D

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Types of data

- Categorical / Nominal (classes)
- Categorical / Ordinal
- Continuous / Interval (e.g. Celsius)
- Continuous / Ratio
- Discrete: binned/grouped data
- Hard data: direct measurements
- Soft data: indirect measurements, very uncertain
- Primary data: variable(s) of interest
- Secondary data: descriptors
- Collective variables
- Latent variables

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Descriptive and Predictive statistics

Estimation

- Process of obtaining the best value or range of a property in an unsampled location
- Local accuracy takes precedence over global spatial variability
- Not appropriate for forecasting

Inference

- Predict unseen samples given assumptions about the population
- Test with a pre-trained model (ML definition)
- Generality versus Accuracy

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Variables and Features, Labels and Instances

Population

Exhaustive, finite list of properties of interest over area of interest.

Generally the entire population is not accessible

Samples/experiments/instances

The set of values and location that have been measured.

How many experiments are needed?

Sampling distribution -(IID ?)

identical and independent distribution The set of values and location that have been measured.

Features

The values to be measured for each sample/experiment/instance.

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Predictors = input variables, X_1, ..., X_M

Response = output variables

Error

Deviation from ... exact value (or expected value, mean value, trend...?)

Errors without definitions are just numbers.

Error

Values, without error, are just number!!

Predictor and Response Features

Given a model $Y = f(X_1, ..., X_M) + e$

!Here and error! But is it even an error?

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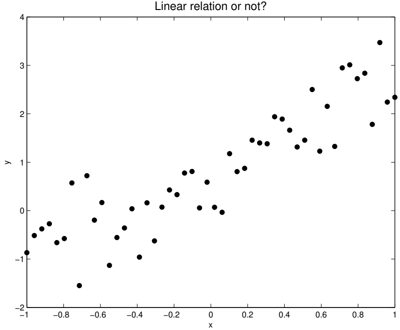
Finding a suitable model

Soft modeling is in most cases based on **multivariate statistical methods**. Many of these methods may be viewed as sophisticated ways of performing curve fitting to data.



What would be the best model?

- Straight?: $y(x) = ax + b$
- Parabolic?: $y(x) = ax^2 + bx + c$
- Trigonometric?: $y(x) = asin(x) + bcos(x)$

Uncertainty Modeling

Given a model, Generate multiple simulation to represent uncertainty

- Realizations: for the same input parameters, different random numbers.
- Scenarios: different input parameters.

Sampling representative.

Random sampling

Each item of the population has an equal chance of being chosen.

- Very expensive
- Mostly not interesting
- Gives some global properties

Bias sampling

Selection of data is (arbitrarily) distorted

- Sample probability bias has to be corrected for
- Might not capture the global picture
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Cognitive biases

- anchoring: The first bits are over-considered
- availability: over-estimating the importance of info
- bandwagon: P increases with the number of people holding a belief
- blind spot: not seen biases
- choice supporting: commitment/decision dependent
- clustering illusion: seeing patterns in random events
- confirmation bias
- conservatism bias
- Recency bias
- Supervision bias
- Many many more!

Bias DO NOT cancel out! They sum up (or multiply?)

Simulations

Process of obtaining one or more values of a property

- Improved Global accuracy
- Better property distributions

Why simulations then?

- We need to capture the full distribution of properties, extremes matter!
- We need more realistic models.

Why not?

- High dimensionality level
- Computationally expensive
- Convergence limitations
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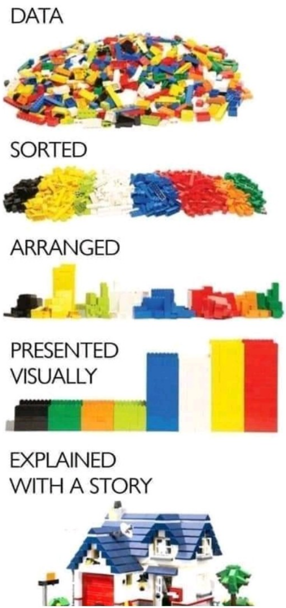
DATA
SORTED
ARRANGED
PRESENTED VISUALLY
EXPLAINED WITH A STORY

Representation

A representation should **capture** the nature of the subject being studied.

Example: If you want to evaluate the 3D structure of a wind turbine, a set of descriptors an be:

1. Blade length
2. Turbine height
3. Geographical position
4. Output power
5. Wind direction

which are two decimal numbers, a 2d tuple, a 1D time series and a 2D time series (or 3D even).

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Comparability

Same meaning **represenations** for different objects (inputs).

Discussion point!

How do we compare two wind turbines accounting for the 5 variables previously introduced?

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Data properties

- All starts from data: what are data-properties?
- Are there such things as good data and bad data?

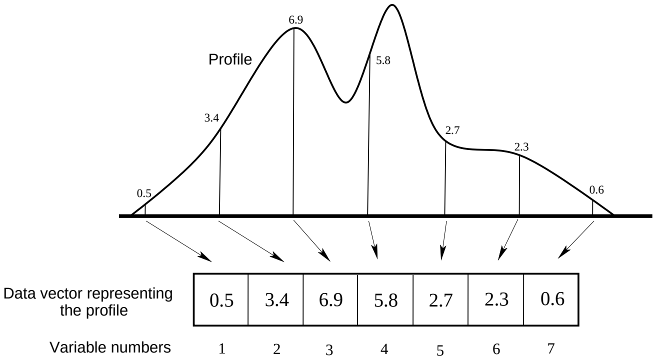
Life lesson (or exam question, same thing ;))

- Data DO NOT always have value.

- TRASH in TRASH out

Sampling point representation (SPR)

- An intuitive way to represent curves and spectra is the **sampling point representation**.
- We sample at regular intervals where each sample point is represented by a variable



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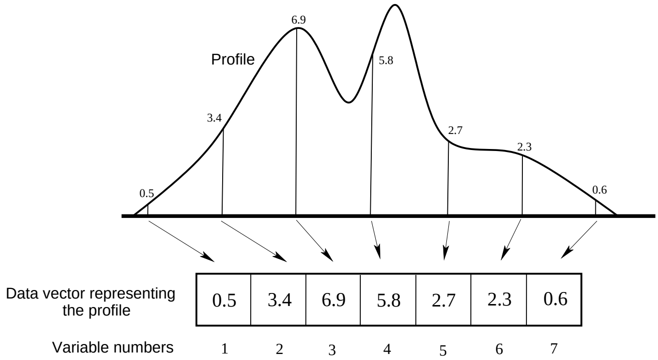

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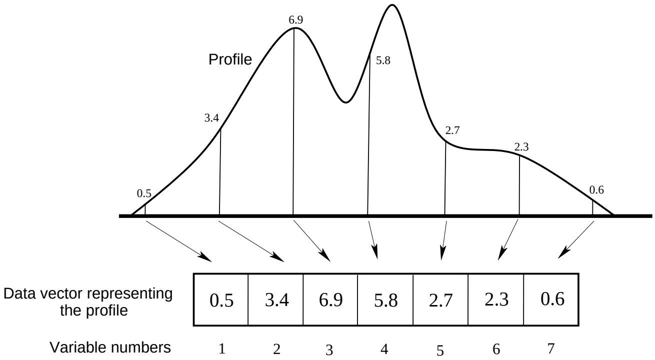

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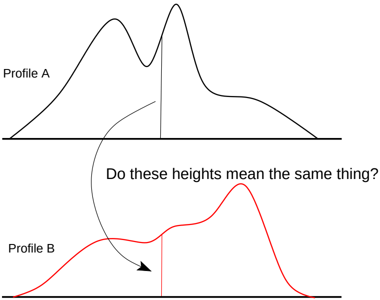

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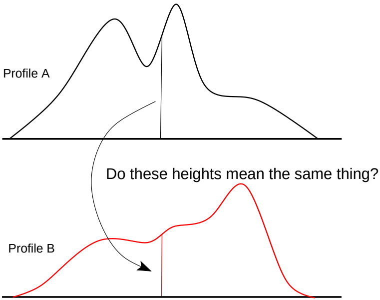

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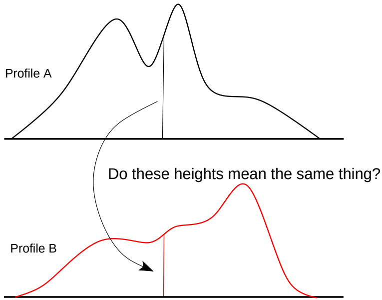

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Data structures

Given a representation, it is then needed to decide on a suitable **data structure** for the problem.

Definition

A data structure is a way of storing and organising data in a computer so that it can be used effectively.

Typical data structures used in data analysis are:

- Data points
- Arrays (vectors, matrices, N-mode (way) arrays)
- Graphs (trees)
- Databases

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Workflow

Data has to be prepared with these steps in mind

1. Plan experiments: Use experimental design to set up experiments in a *systematic* way
2. Pre-processing: Is there systematic variation in the data which should be removed Can cross-checking/validation procedures be designed?
3. Examine the data: Look at data (tables and plots). Strange behaviours? Smooth behaviour? WARNING!
4. Define desired model outcomes (speed, accuracy, false positive/negatives rate)
5. Estimate and validate model: What do the results tell us? Is the generated model general (valid for future sampling)?
6. Apply model to unknown samples

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Spatial and Temporal Data

Statistics is collecting, organising, and interpreting data

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3. the different relative value and precision of the data.

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Actual data

The data matrix is an extremely common data structure.

$$X = \begin{bmatrix} 95 & 89 & 82 \\ 23 & 76 & 44 \\ 61 & 46 & 62 \\ 49 & 2 & 79 \end{bmatrix}$$

In python these can be saved as

- lists (vanilla python)
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- pandas dataframes

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Nomenclature Reminder

There are different conventions. Commonly we will construct data matrix such that:

- Rows are called instances, objects or samples.
- Columns are called features, variables.

One can think of each row to be an experiment, and the rows its properties. Each row (experiment, object, sample, ...) is thus a list of values, one for property.

Note

Mathematically speaking, this is just a notation. As long as one keeps track and is consistent, columns can be used as rows and vice versa.

A quick example

Environmental measurements of rivers. The features (properties) can be:

- pH
- Temperature
- Concentration of pollutants
- Flow rate
- water speed

The experiments/observations/sample can be:

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