COMS30035, Machine learning: Machine Learning Concepts

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18th September 2025

Acknowledgement

- These slides are adapted from ones originally created by Rui Ponte Costa and later edited by Edwin Simpson.

Agenda

- The different forms of machine learning:
  - Unsupervised learning
  - Supervised learning
  - Reinforcement learning
- Other important concepts in ML:
  - Overfitting
  - Model selection
  - The curse of dimensionality
  - No free lunch theorem
  - Parametric vs non-parametric models

The different forms of machine learning

- ML attempts to learn **models** of the world
  - Usually with many simplifications
  - Models are a way of understanding how **input** data relates to the **outputs**
  - E.g., a function that maps weather observations to predictions

The different forms of machine learning

- ML attempts to **learn** models of the world
  - Many different flavours of data are available!
- The data available defines which form of learning we can use
- However, the principle is always the same: model the data..
  - ...the model assumptions and data structure vary

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Unsupervised learning

Only the input data is provided and models learn to extract patterns from the data.
Example tasks [1]:

- Clustering: grouping similar items together (e.g., K-means, unsupervised HMM)
- Dimensionality reduction (e.g. PCA): finding a simplified representation of input data with fewer dimensions
- Density estimation (mixture models, language models): used to estimate the probability distributions from data

[1] Note that virtually all models that do not use explicit teaching signals, such as targets/labels or rewards are unsupervised.

Supervised learning

Each input is paired with an output – a "label" or "target" – and the model is trained to minimise the error (difference) between its output and the target.

Example tasks:

- Regression: numerical outputs (e.g. air temperatures over time)
- Classification: category labels (e.g. dog or bagel?)

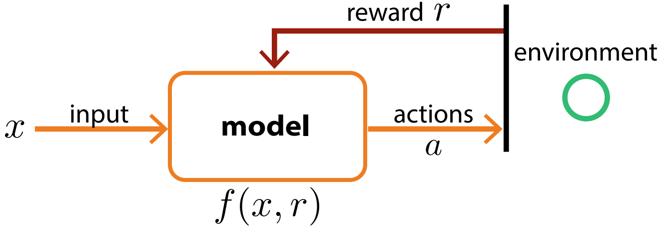
Many learning methods can be used for both regression and classification:

- Supervised neural networks
- Support vector machines
- Decision trees

Reinforcement learning

The correct outputs are not given, but the model receives a reward (or punishment) depending on its actions.

RL deals with dynamic environments where agents carry out sequences of actions. It is inspired by animal behaviour. RL is seen as a field on its own – *we do* **not** *teach RL on this unit*.



Examples:

- Temporal difference learning
- Deep reinforcement learning (uses neural networks)

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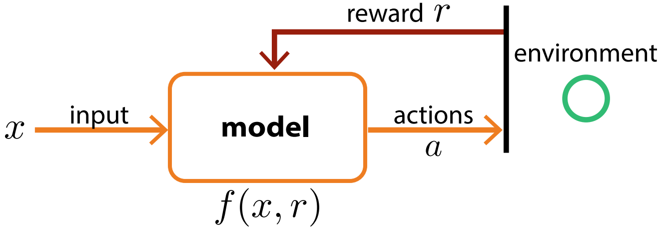


Examples:

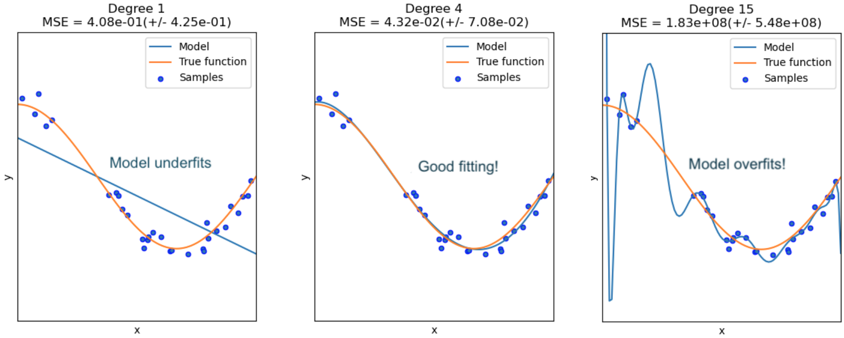
- Temporal difference learning
- Deep reinforcement learning (uses neural networks)

Underfitting vs overfitting

Underfitting: A model that is too simple – it should be as "simple as possible, but no simpler."[2]

Overfitting: A model that fits minor variations or noise; highly flexible models are particularly prone to overfitting.

Example from *scikit-learn* (click here):



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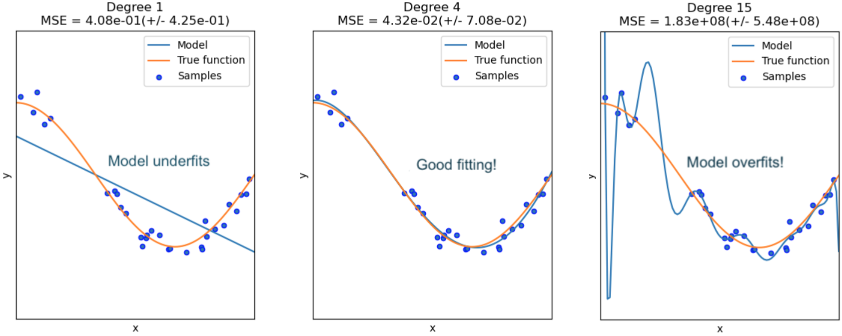

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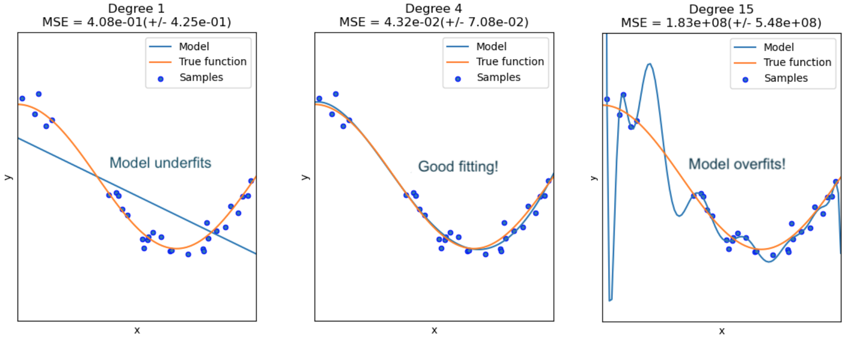

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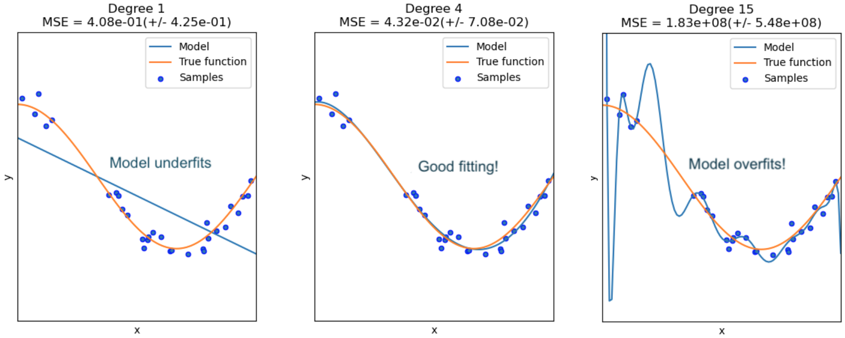

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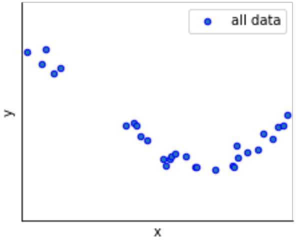
Model selection

There are an infinite number of models, how do we choose just one?
Answer: We perform model selection to reduce under/overfitting.[3]

A common method is to *split the dataset*. Let's look again at the data used in the previous slide

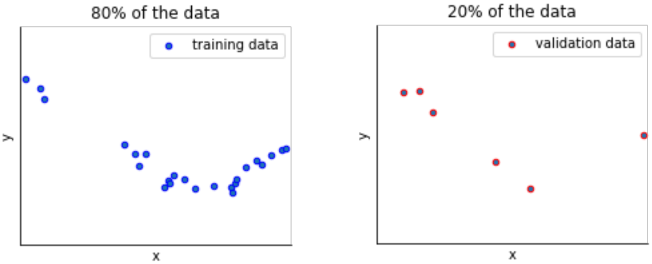


[3]Note that models that overfit or underfit fail to **generalise** to new data, this idea underlies model selection.

Model selection

Let's split the full dataset into:

- **Training dataset**: Used for training/optimising your model (e.g. use 80% of the full dataset)
- **Validation dataset**: Used *only* for validating your model (e.g. use 20% of the full dataset)



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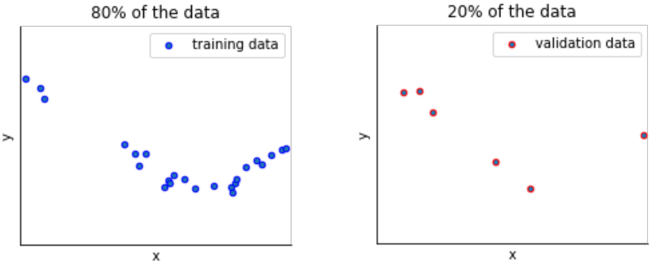
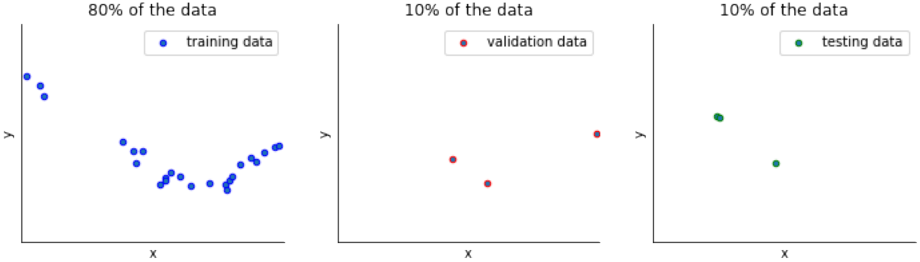


Model selection

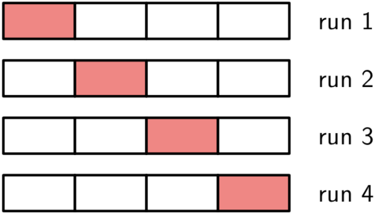
- **Testing dataset**: Used to test the model for general fitting quality after the optimisation procedure has finished (e.g. use 10% of the full dataset).



Model selection

However, simply splitting the data means that we end up with less data for training the model. A solution is to cycle over multiple subsets of the data using *cross-validation*.

- **Cross-validation**: The original data is split into S groups so that $(S-1)/S$ data is used for training. It is common to set S to a relatively low number, e.g. $S = 4$, which gives 4-fold cross validation using 3 (75% of the data) subsets for training (white blocks) and 1 for validation (red block) for each run.[4]



[4] If $S = N$ where N is the full number of data samples it gives the *leave-one-out* method.

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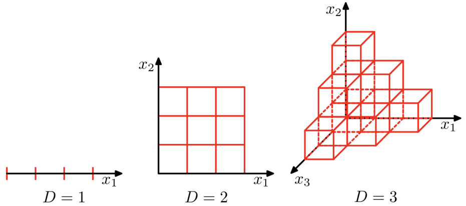
  - **The curse of dimensionality**
  - **No free lunch theorem**
  - **Parametric vs non-parametric models**

Curse of dimensionality in ML

1D and 2D spaces can be covered by data easily, but for higher dimensions this is no longer feasible.

- If we were to divide the space into cells we would quickly need an exponentially large quantity of data to fill in all cells (see schematic below).
- However, its often possible to find effective algorithms for two reasons (Bishop book):
  - Data is often restricted to specific regions of the much bigger spaces – i.e. effective dimensionality is much smaller.
  - Data typically has smoothness properties – i.e. small changes in the input variables will lead to small changes in the output variables.



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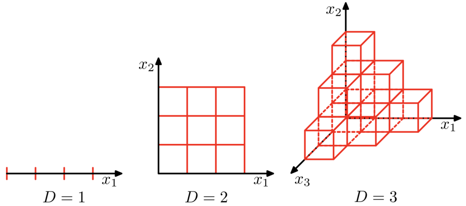

No free lunch theorem

All models are wrong, but some models are useful. — George Box 1976

- Using model selection we can obtain a *good model*.
- *But* there is no universally best model – **no free lunch theorem** (Wolpert 1996).
- Why? Models always make assumptions and these often do not generalise across domains – different domains need different models.

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- **Parametric**: Model assumes a fixed number of parameters θ.
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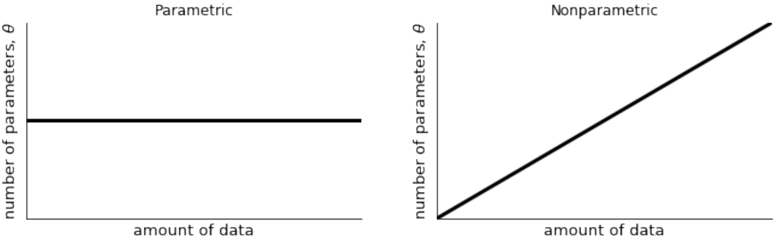

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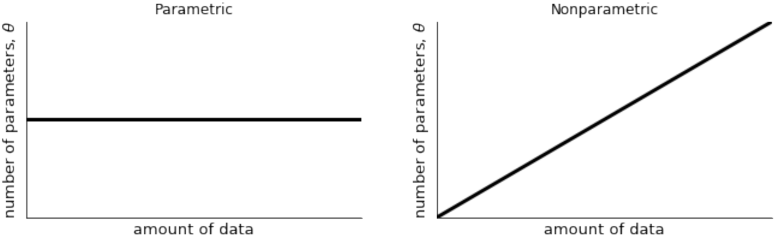

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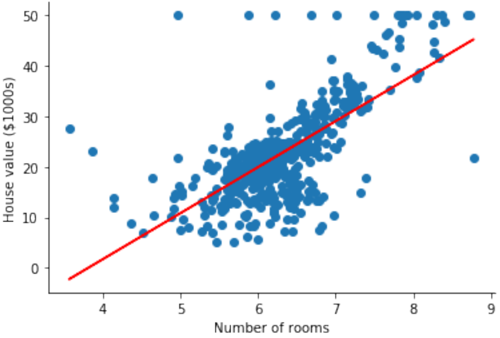
Parametric models

- **Pros**: Simpler, fast to fit and may require less data.
- **Cons**: Complexity is fixed. Simple models are better for simpler problems/datasets.

Example: Linear regression model $y = ax + b$ assumes 2 parameters $\theta = \{a, b\}$, where a is the slope and b the y-intercept.



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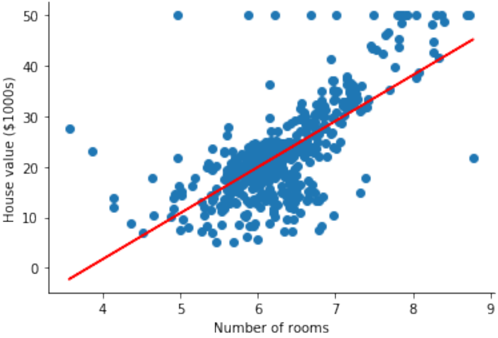

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- **Pros**: Flexible (i.e. can infer which functions to use), weak assumptions, can give better models.
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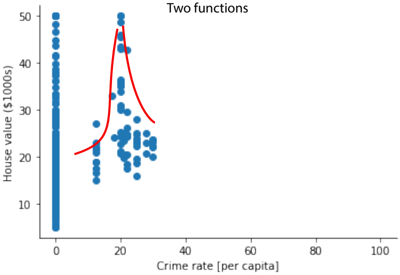
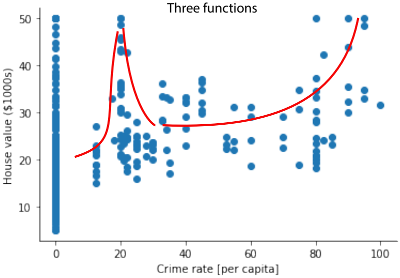
Example: Nonparametric regression with an algorithm[6] that automatically detects which polynomial functions to use.





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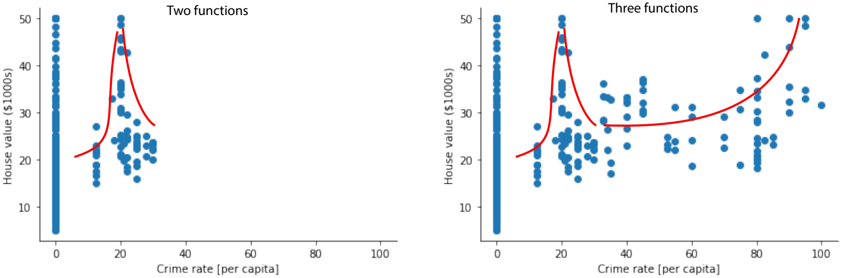

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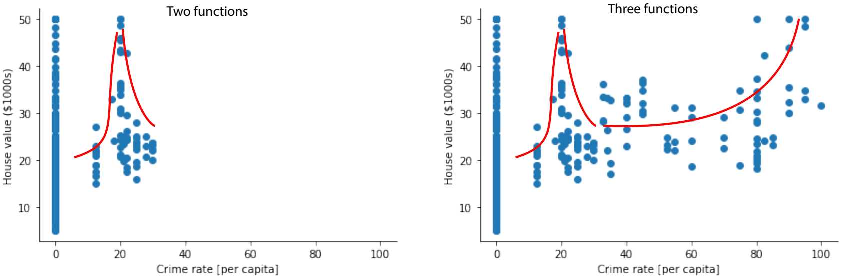

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Reading

- Bishop §1.1–§1.4. (§1.2 is about Probability Theory which we did not cover here but is useful ‘revision’.)
- The whole of Murphy Chapter 1 is a good read, but if you wish to just focus on this lecture’s material look at Murphy §1.1-§1.2.

Problems and quizzes

- No problems.
- Quizzes:
  - Week 1: Machine Learning Concepts