COMS30035, Machine learning: Machine Learning Concepts

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Acknowledgement

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

Textbooks

We will go over ML concepts following Chapter 1 of both textbooks:

- Bishop, C. M., Pattern recognition and machine learning (2006). Available for free here.
- Murphy, K., Probabilistic Machine Learning: An Introduction (2022). This book is also freely available here.

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

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  - 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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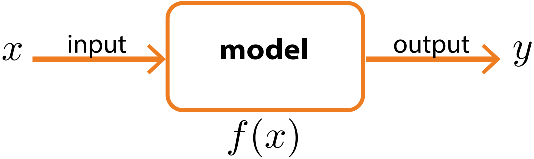
Unsupervised learning

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 probabilities of input data points

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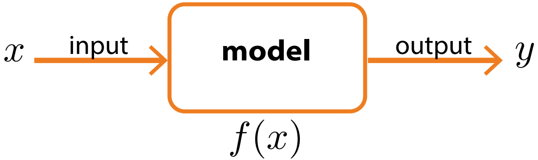

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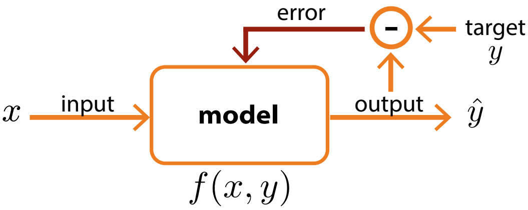

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Many learning methods can be used for both regression and classification:

- Supervised neural networks
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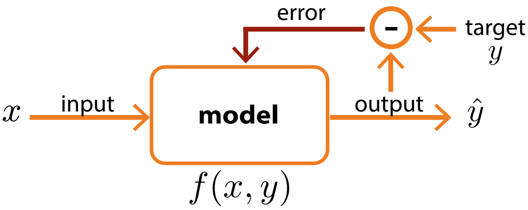

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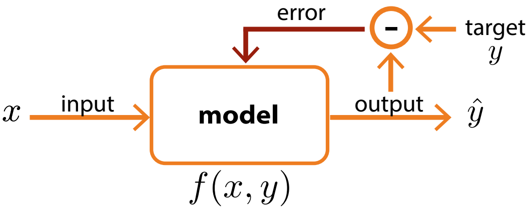

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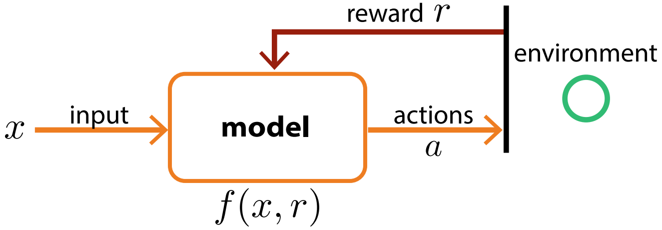
The correct outputs are not given, but the model receives a reward (or punishment) depending on its actions.

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:

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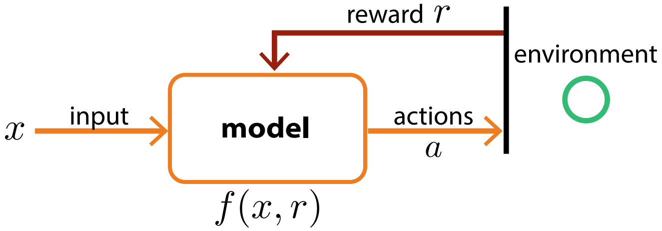

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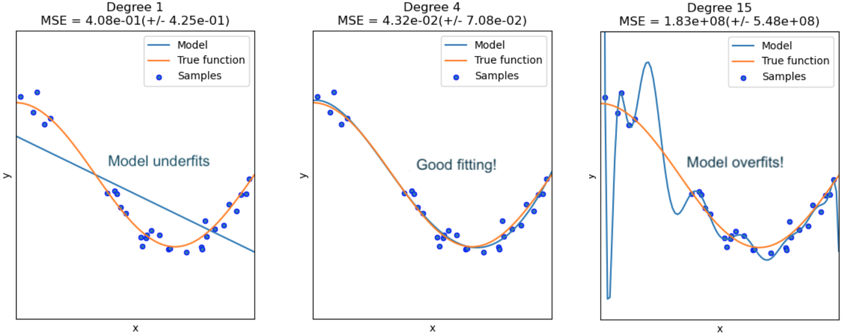
Underfitting vs overfitting

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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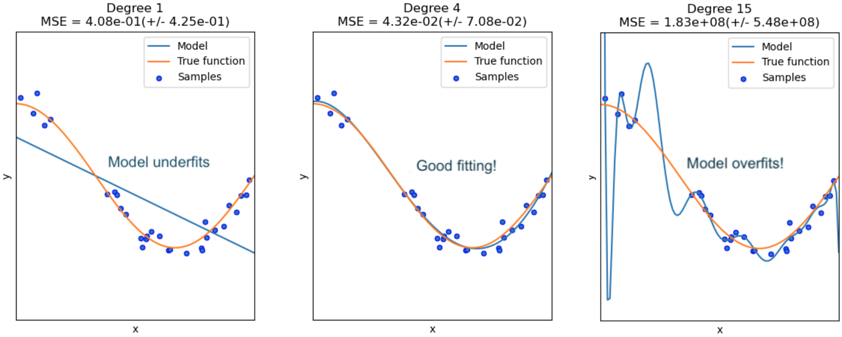

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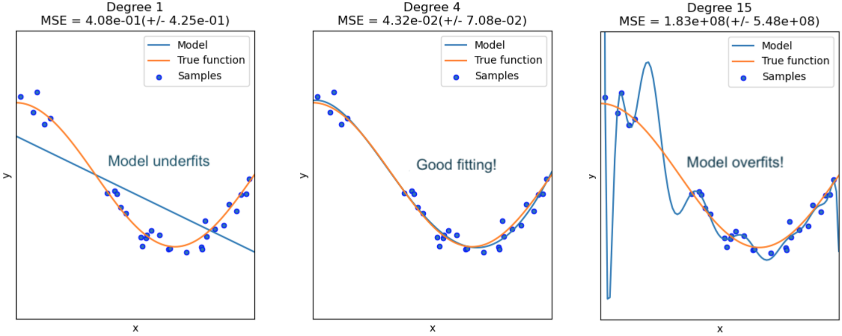

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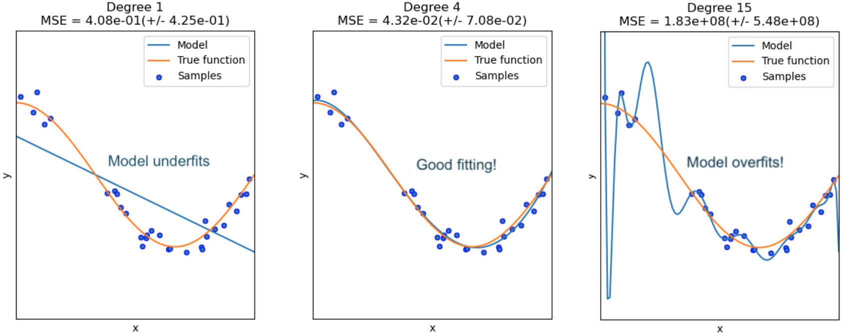

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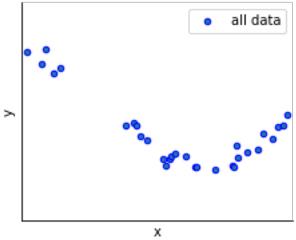
Model selection

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

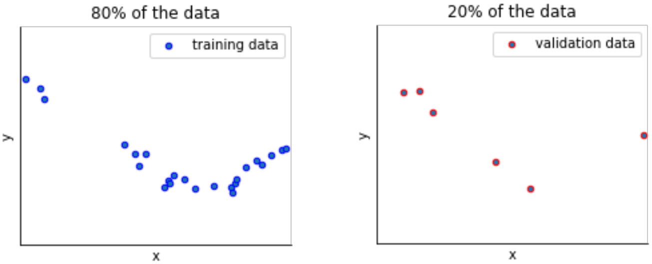


[3]Note that models that overfit or underfit fail to **generalise** to new data, this idea underlies model selection.

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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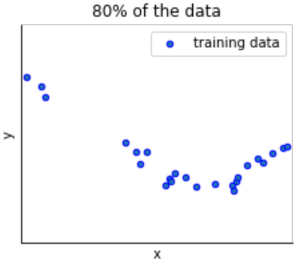


Model selection

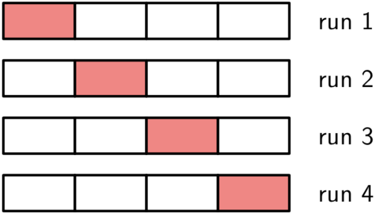
Relying only on the validation dataset to select our models can lead us to overfit to that data, in particular for small datasets and iterative methods. So it is often common to use a third subset, the *testing dataset*.

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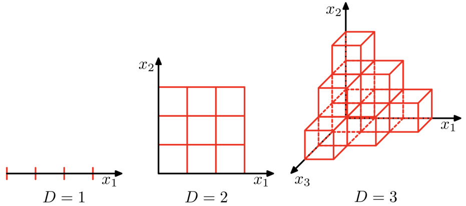
  - **The curse of dimensionality**
  - **No free lunch theorem**
  - **Parametric vs non-parametric models**

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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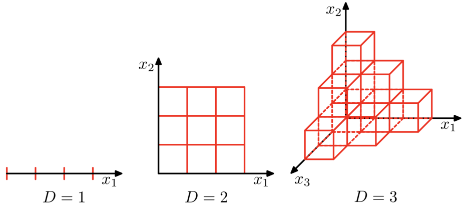

No free lunch theorem

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).
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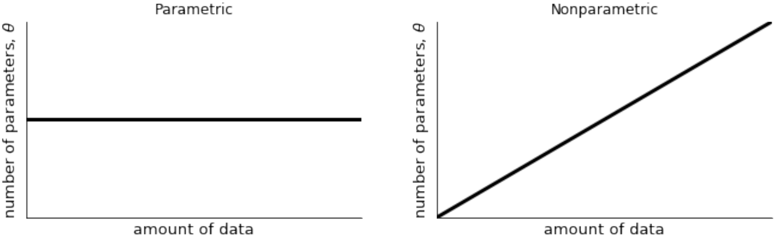

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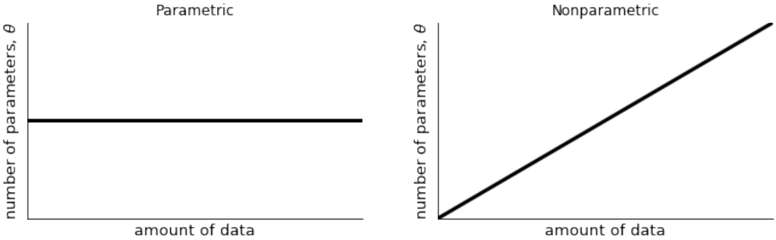

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Parametric models

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

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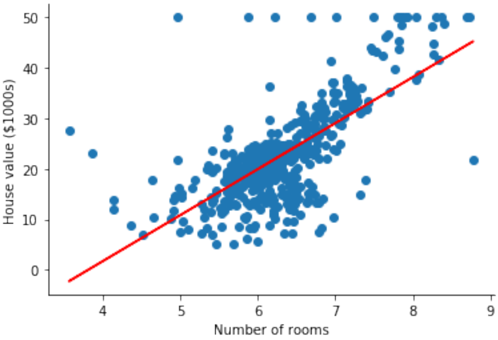

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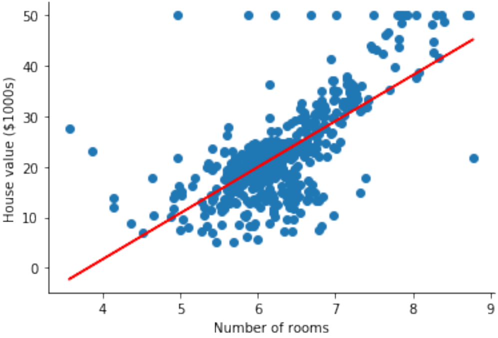

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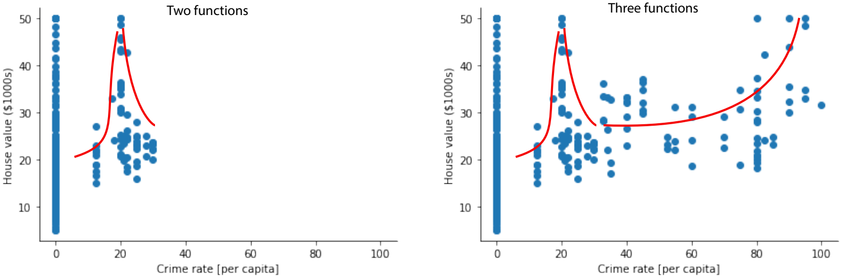

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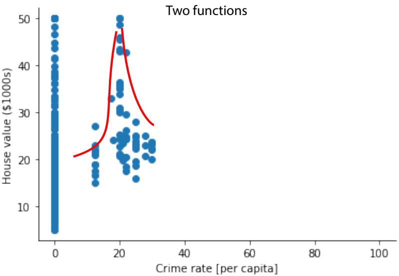

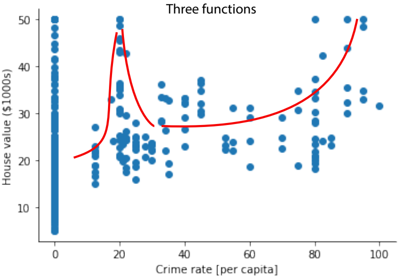

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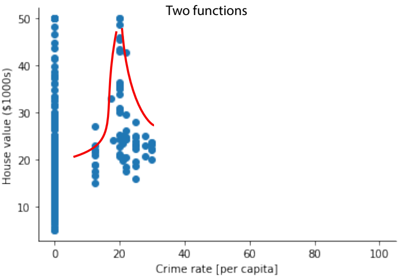

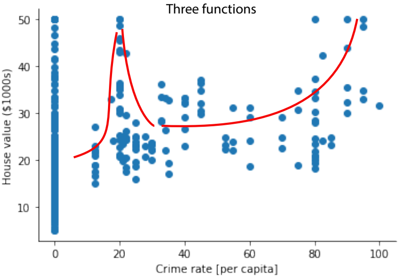

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