COMS30035, Machine learning:

Key ML concepts

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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., Machine learning a probabilistic perspective (2012). The book is also freely available here.

Agenda

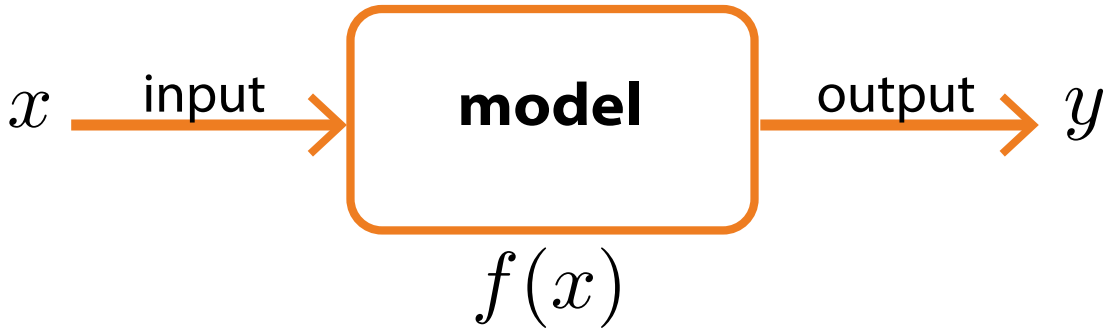
- The different forms of machine learning:
  - Unsupervised learning
  - Supervised learning
  - Reinforcement learning
- Other important concepts in ML:
  - Overfitting
  - Model selection
  - The curse of dimentionality
  - No free lunch theorem
  - Parametric vs non-parametric models

The different forms of (machine) learning

- ML attempts to learn models of the world
  - The world comes in all flavours of data!
- The data available defines which form of learning we can use
- Although, the principle is always the same: model the data..
  - ..the model assumptions and data structure varies.

Unsupervised learning

In UL models only rely on the input data directly and extract insights/patterns from the data.



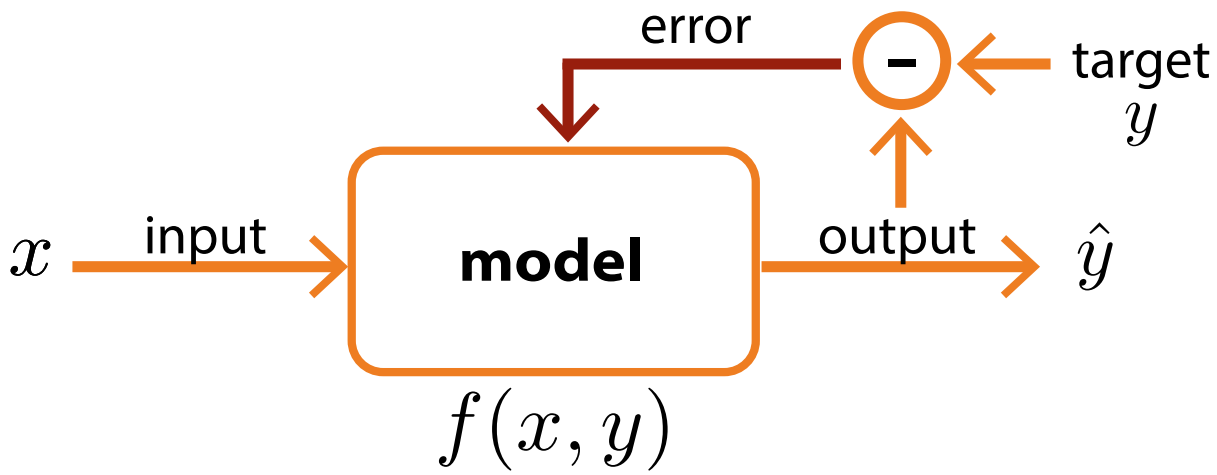
Examples [1]:

- Linear or nonlinear regression
- Latent models (PCA, ICA)
- Mixture models
- Unsupervised hidden markov models
- Unsupervised neural networks

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

Supervised learning

In SL models rely on specific labels or targets (e.g. from last lecture: is this a dog or a bagel?). This in turn means that models are trained to minimise an error signal (e.g. calculated as the difference between its output and the desired target).

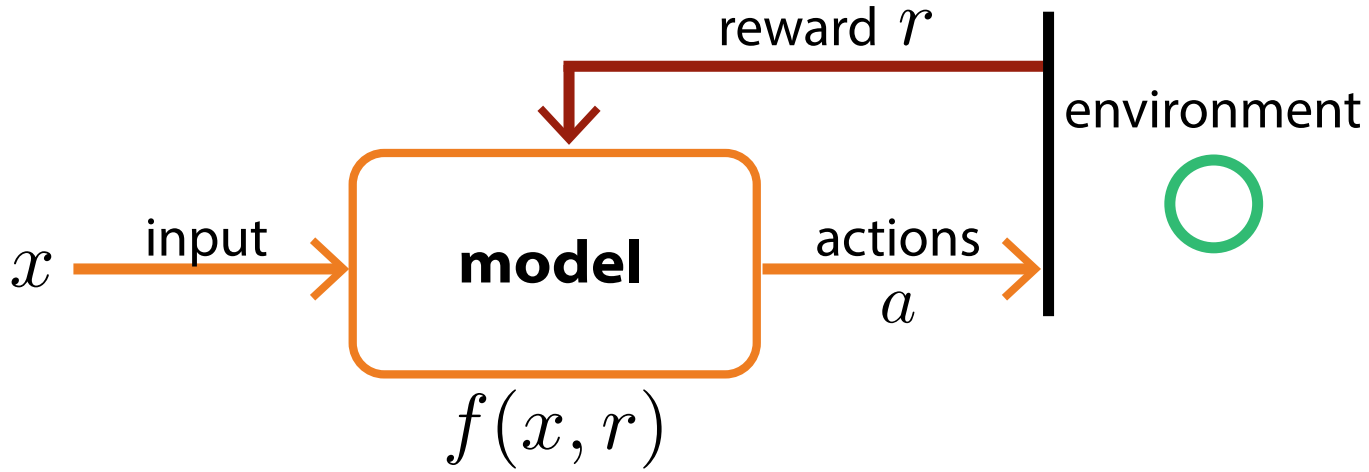


Examples:

- Supervised neural networks
- Support vector machines
- Decision trees

Reinforcement learning

RL deals with dynamic environments and inspired on animal behaviour – algorithms are designed to deal explicitly with an environment in which rewards (and punishments exist). RL is seen as a field on its own – *we do **not** teaching RL methods on this unit*.



Examples [2]:

- Temporal difference learning
- Deep reinforcement learning (uses neural networks)
- Key to develop truly autonomous systems

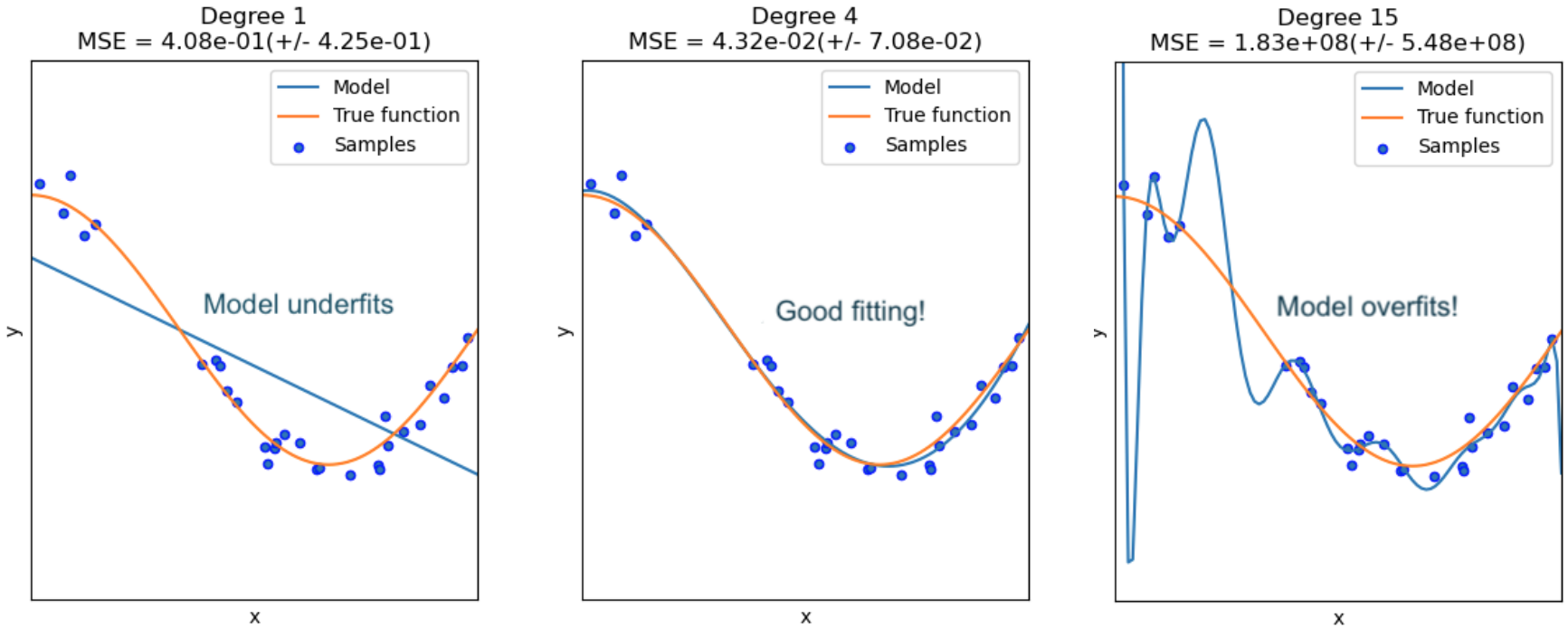
[2] If you would like to learn more see Information Processing and the Brain in your 4th year.

Underfitting vs overfitting

Underfitting: A model that is too simple – it should be as "simple as possible, but no simpler."[3]

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

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

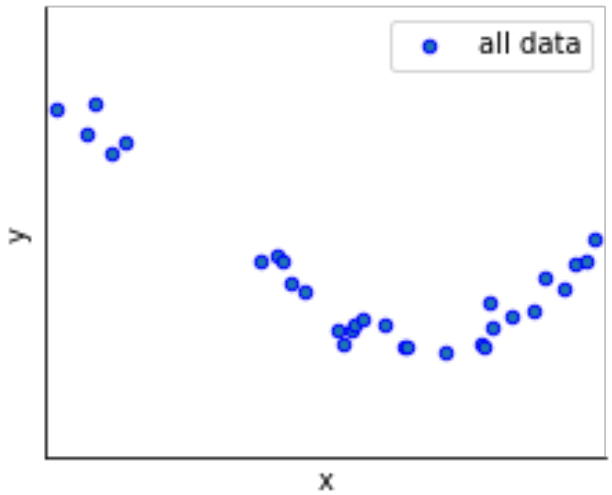


[3] As Einstein used to say when formulating theories "Everything should be made as simple as possible, but no simpler."

Model selection

There is an infinity number of models, how do we choose just one?
Answer: We perform model selection to reduce under/overfitting. [4].

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

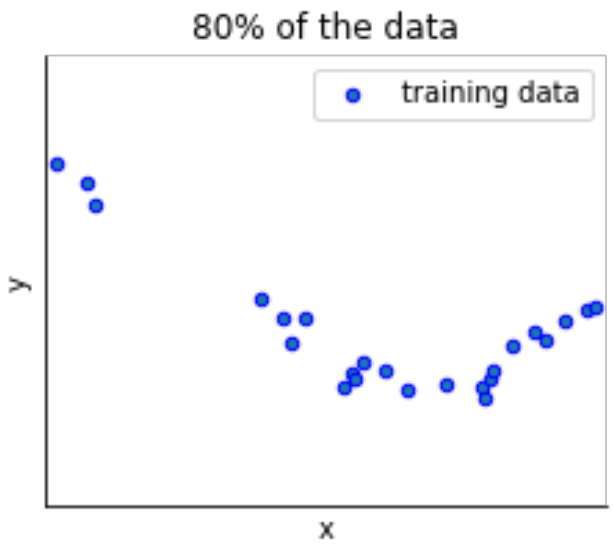


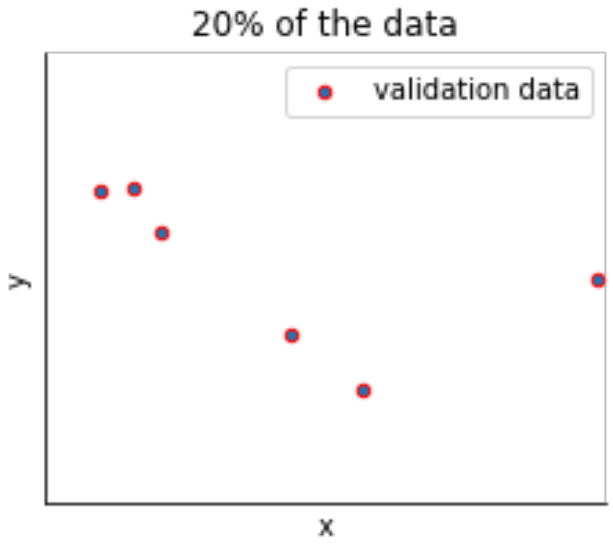
[4]Note that models that overfit or underfit fail to **generalise** to new data, this idea underlies model selection.

Model selection

Lets 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)

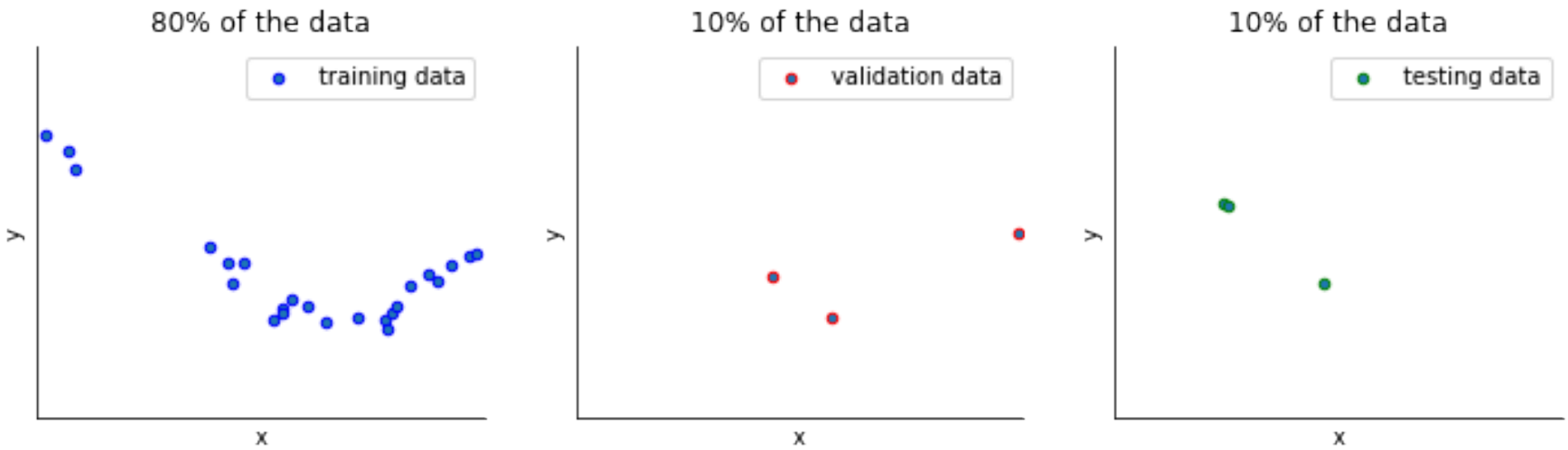




Model selection

Relying only on the validation dataset to select our models can lead for us 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*.

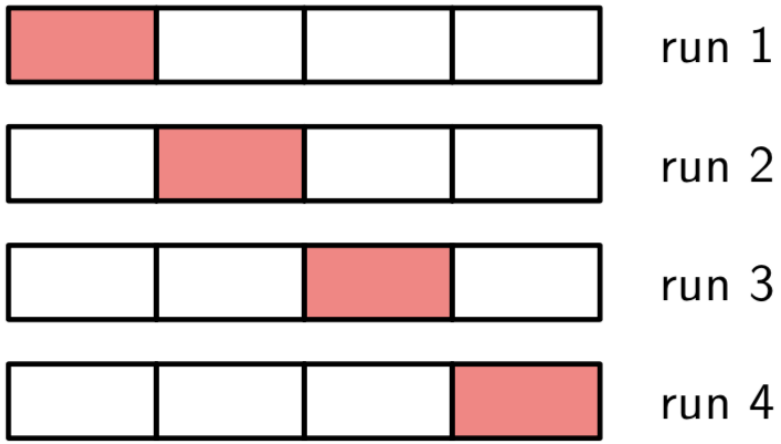
- **Testing dataset**: Used to test the model for general fitting quality after the optimisation procedure has finished (e.g. use 10% of the full dataset).



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 [5]:



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

Quiz time!

Go to Blackboard unit page » Quizzes » Lecture 2

[Should take you less than 3 minutes]

Agenda

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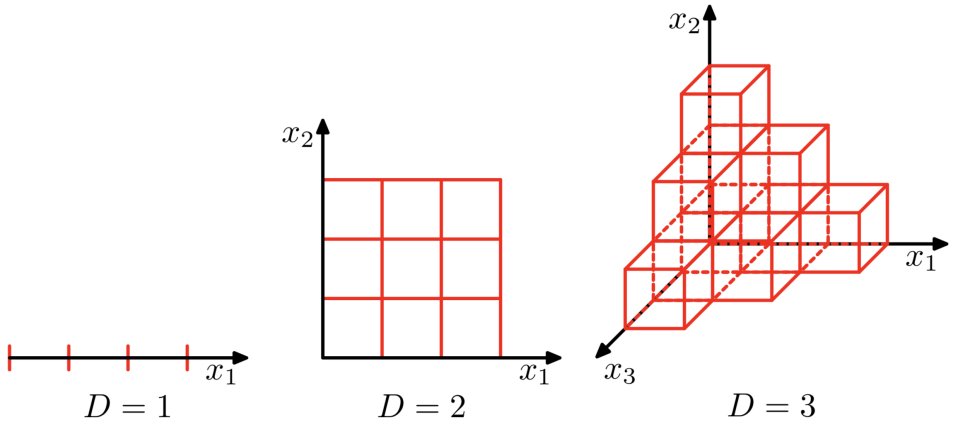
  - Supervised learning
  - Reinforcement learning
- Other important concepts in ML:
  - Overfitting
  - Model selection
  - **The curse of dimentionality**
  - **No free lunch theorem**
  - **Parametric vs non-parametric models**

Curse of dimentionality 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 dimentionality 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.



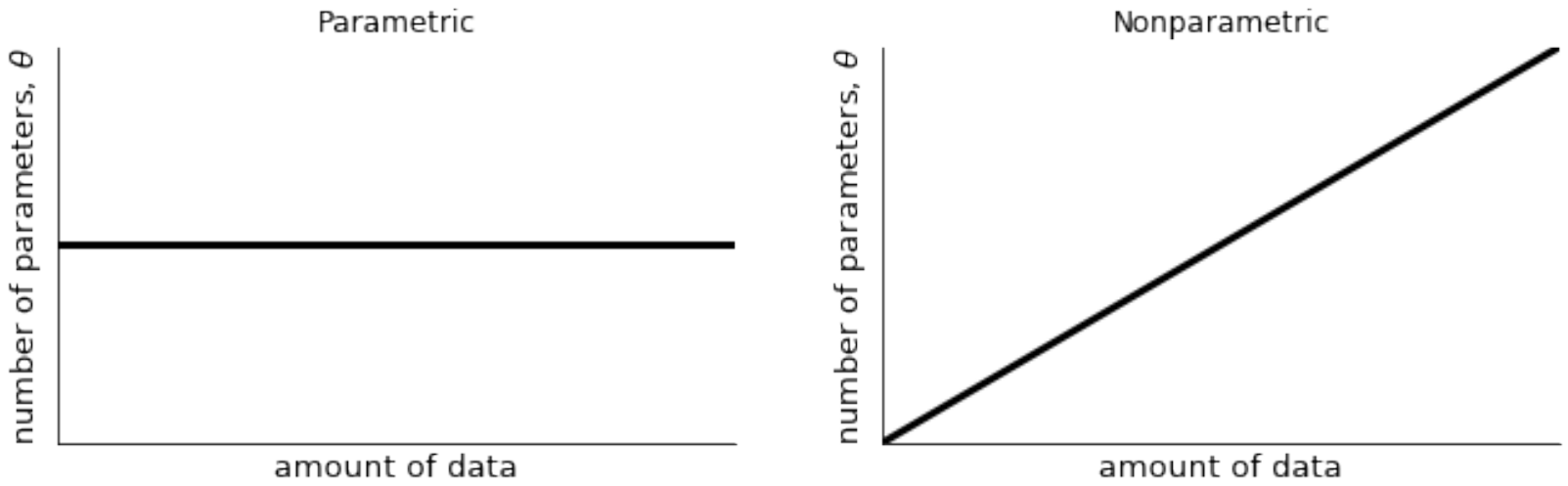
No free lunch theorem

All models are wrong, but some models are useful. — George Box 1987

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

Parametric vs non-parametric models

- **Parametric**: Model assumes fixed number parameters θ.
- **Non-parametric**: Model parameters θ grows with the amount of data.[6]

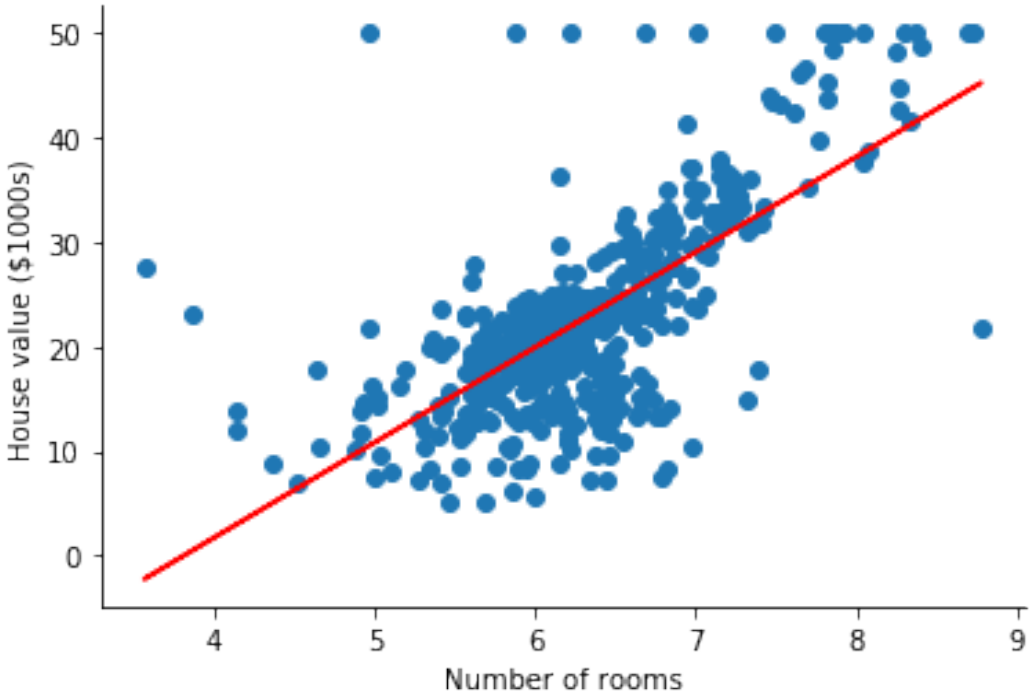


[6] Most nonparametric models are hybrid models with parametric (non-flexible) components.

Parametric models

- **Pros**: Simpler, fast to fit and require less data.
- **Cons**: Limited and better for simpler problems/datasets.

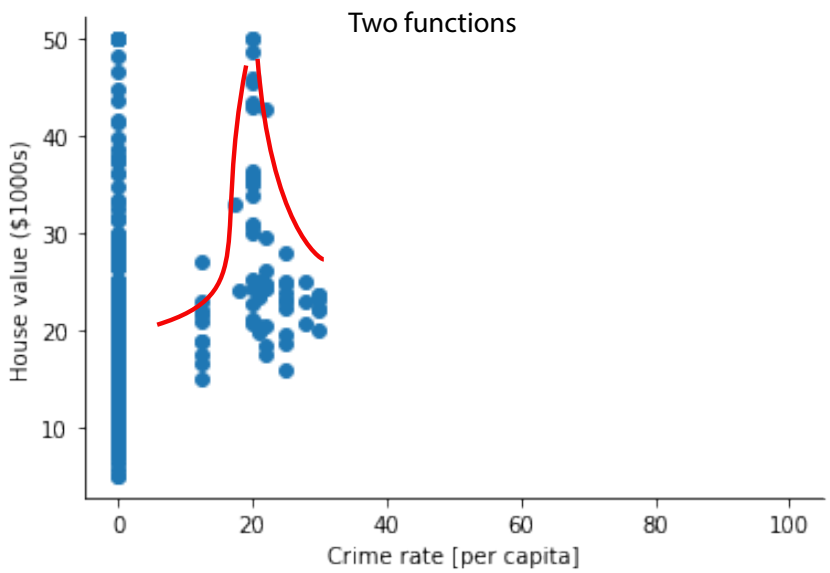
Example: Linear regression model $y = ax + b$ assumes 2 parameters $\theta = \{a, b\}$, where a is the slope and b the y-intercept.

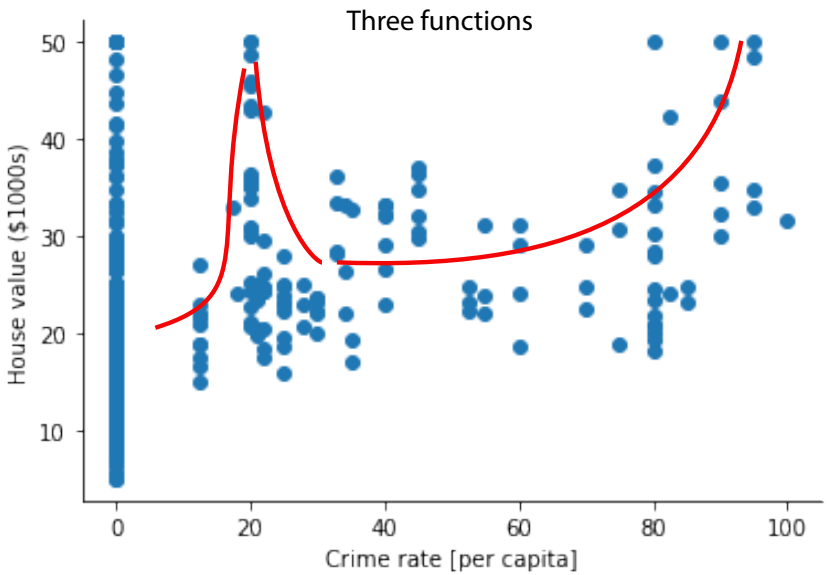


Non-parametric models

- **Pros**: Flexible (i.e. can infer which functions to use), weak assumptions, can give better models.
- **Cons**: Need more data, slower to train (more parameters), risk of overfitting.

Example: Nonparametric regression with an algorithm[7] that automatically detects which polynomial functions to use.





[7] Note that this is an hypothetical algorithm to illustrate the increase in number of parameters as a function of data.

Tasks

- Live lecture week 2 (Tue 9-10): Questions about the ML concepts, linear regression and nnets
  - You should use the Teams QA>Ask Question system to ask question before hand.

- Next lab (Week 2): Linear and non linear regression, nnets and SVMs
  1. Join meeting on your Bubble [from 10am on Thu]
  2. See link to lab 2 on BB