

# MSc Data Mining

## Topic 03 : Data Modelling - Introduction

### Part 01 ; Data Modelling - Introduction

Dr Bernard Butler and Dr Kieran Murphy

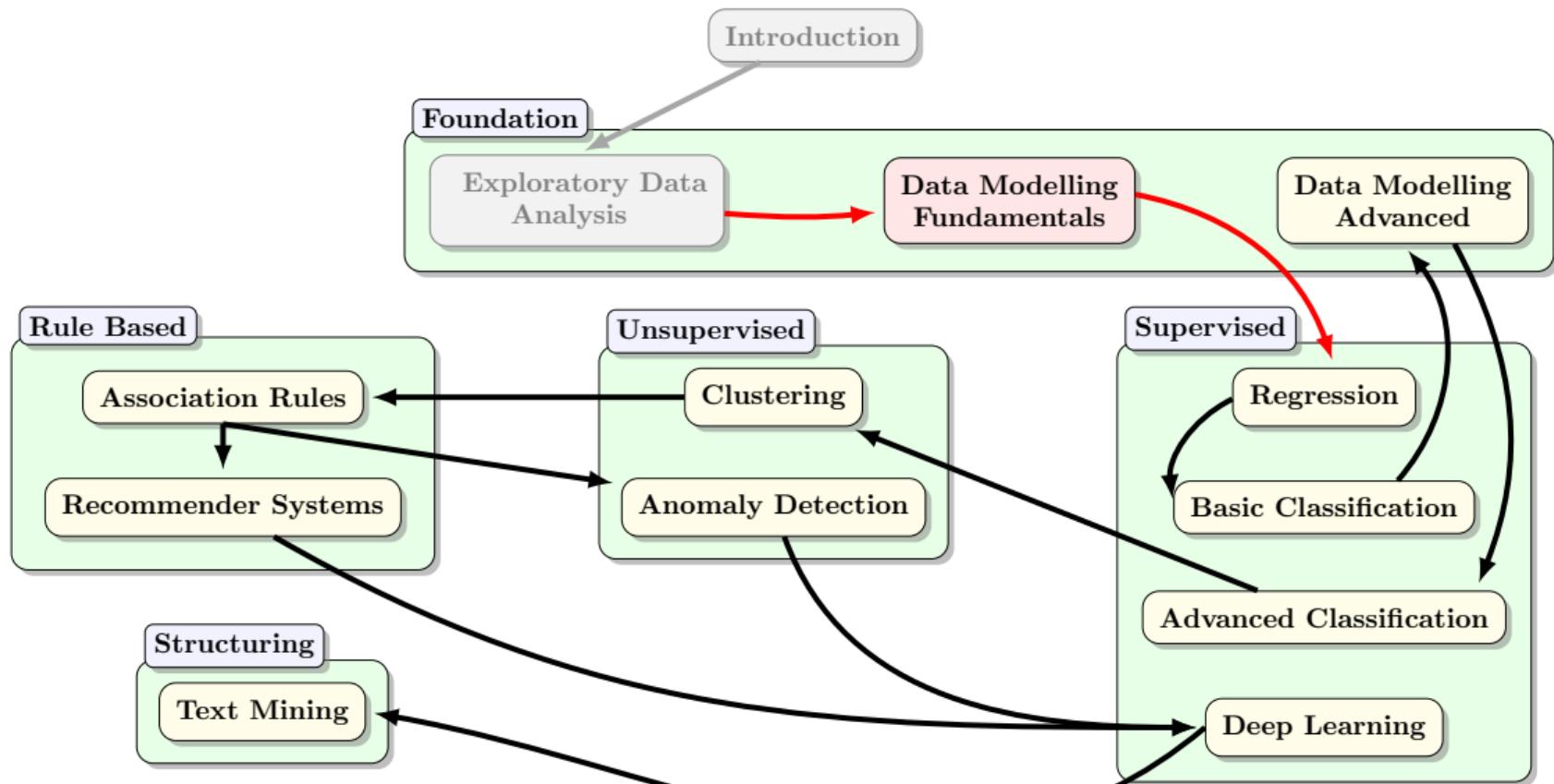
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Spring Semester, 2023

#### Outline

- Components of a machine learning problem
- Machine learning concepts and notation
- Bias vs variance
- Learning curves
- Regularisation

# Data Mining (Week 3)



# Outline

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# Three Components of a Machine Learning Problem

It is easy to get lost among the multitude of concepts to address and the choices one needs to make when given data mining problem. A good decomposition is the following:

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
<i>K</i> -nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search
Hyperplanes	Likelihood	Branch-and-bound
Naive Bayes	Posterior probability	Continuous optimization
Logistic regression	Information gain	Unconstrained
Decision trees	K-L divergence	Gradient descent
Sets of rules	Cost/Utility	Conjugate gradient
Propositional rules	Margin	Quasi-Newton methods
Logic programs		Constrained
Neural networks		Linear programming
Graphical models		Quadratic programming
Bayesian networks		
Conditional random fields		

# Three Components of a ML Problem — Representation

Representation	Evaluation	Optimization
Instances  K-nearest neighbor  Support vector machines	Accuracy/Error rate  Precision and recall  Squared error	Combinatorial optimization  Greedy search  Beam search

**Representation** refers to formulating the problem as a machine learning problem — typically a **classification** problem, a **regression** problem or a **clustering** problem.

- How do we represent the input?
- What **features** to use?
- How do we learn additional features?
- With each type of problem, we have multiple subtypes:  
For example which classifier? a **decision tree**, a **neural network**, a **support vector machine**, etc.

# Three Components of a ML Problem — Evaluation

Representation	Evaluation	Optimization
Instances  K-nearest neighbor  Support vector machines	Accuracy/Error rate  Precision and recall  Squared error	Combinatorial optimization  Greedy search  Beam search

**Evaluation** refers to an **objective function** or a **scoring function**, to distinguish a good model from a bad model.

- For a classification problem, we need this function to know if a given classifier is good or bad. A typical function can be based on the number of errors made by the classifier on a test set, using precision and recall.
- For a regression problem, it could be the squared error, or likelihood. Do we include regularisation? etc

# Three Components of a ML Problem — Optimisation

Representation	Evaluation	Optimization
Instances $K$ -nearest neighbor Support vector machines	Accuracy/Error rate Precision and recall Squared error	Combinatorial optimization Greedy search Beam search

**Optimisation** is concerned with searching among the models in the language for the highest scoring model.

- How do we search among all the alternatives?
- Can we use some greedy approaches, branch and bound approaches, gradient descent, linear programming or quadratic programming methods.

# Taxonomy of Machine Learning Models ...

## ... by Intuition/Motivation

- **Geometric models** use intuitions from geometry such as separating (hyper-)planes, linear transformations and distance metrics.
- **Probabilistic models** view learning as a process of reducing uncertainty, modelled by means of probability distributions.
- **Logical models** are defined in terms of easily interpretable logical expressions.

## ... by Algorithmic Properties

- **Regression models** predict a numeric output.
- **Classification models** predict a discrete class value.
- **Neural networks** learn based on a biological analogy
- **Local models predict** in the local region of a query instance.
- **Tree-based models** (recursively) partition the data to make predictions.
- **Ensembles** learn multiple models and combine their predictions.

## ... by Fixed/Variable Number of Parameters

- **Parametric models** have a fixed number of parameters.
- In **non-parametric models** the number of parameters grows with the amount of training data.

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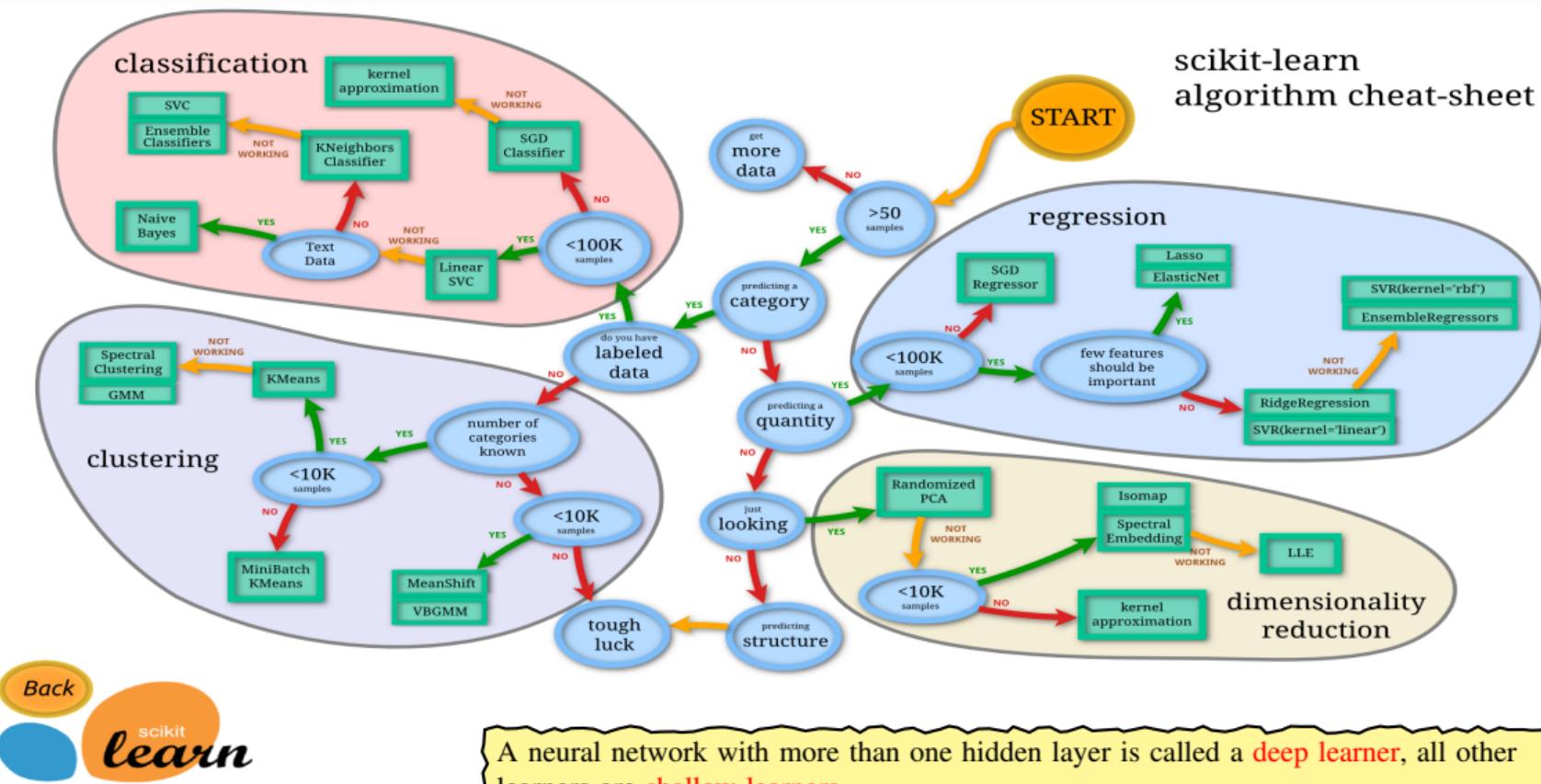
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# Aside: Scikit-learn Flowchart of Models (Shallow Learners)



# Statistical Models vs Machine Learning Models

## Data

### Statistical Models

- Usually small (< 1000 observations)
- Low dimension (< 10 variables)
- Can have detailed understanding of data
- Data is clean — human has looked at each data point

## Models

### ML Models

- Can be huge (million+ observations)
- Large dimension (1000+, more for vision)
- Too large for human to parse / understand
- Data not clean — humans can't afford to understand/fix each point

## Validation

- Simple models — complexity limited by theory
  - Detailed/complex statistical assumptions re data
  - Model known, and data is carefully examined to verify assumptions.
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- Evaluation based on theoretical estimates under stated statistical assumptions
  - Analysis of errors using theoretical distributions

Statistics would be very different if it had been born after the computer instead of 100 years before

- “No” upper limit on model complexity
  - Fewer statistical assumptions on data
  - Don’t know right model? No problem! have multiple models and vote/weight results
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- Use empirical evaluation methods instead of theory—how well does it work on **unseen** data?
  - Don’t estimate expected error, measure it from **unseen** data.

Splitting data into train+test(+validation) is vital

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# Dataset Terminology / Notation

PassengerId	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked	Survived
1	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	Nan	S	0
2	1	Cumings, Mrs. John Bradley (Florence Briggs Th... e)	female	38.0	1	0	PC 17599	71.2833	C85	C	1
3	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	Nan	S	1
4	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S	1
5	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	Nan	S	0
6	3	Moran, Mr. James	male	Nan	0	0	330877	8.4583	Nan	Q	0
7	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	51.8625	E46	S	0
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11	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16.7000	G6	S	1

- A labeled dataset consists of  $m$  rows  $\times$   $(n + 1)$  columns / variables.
- Use bold to represent vectors and matrices.
- Use subscripts to indicate particular **feature / attribute / column** .....  $x_j$
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*m* observations / instances / cases / rows

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*X*

*y* target

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# Aside: A reminder of functions from the past ...

Recall the formula for the line:

$$y = \underbrace{m}_{\text{slope}} x + \underbrace{c}_{\text{intercept}}$$

where given coefficients  $m \neq 0$  and  $c$ .

Examples include

$$y = 3x - 3, \quad y = -1.5x + 4, \quad y = 5x, \quad \dots$$

Now consider the collection of all possible lines — this gives us the **set/family of linear functions**, i.e., all functions of the form



comma separator between inputs and between parameters + semicolon between input(s) and parameter(s)

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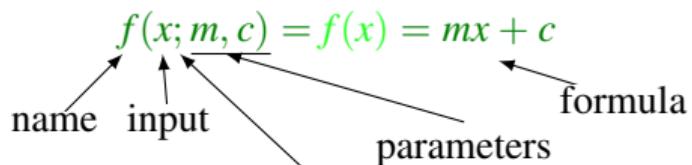
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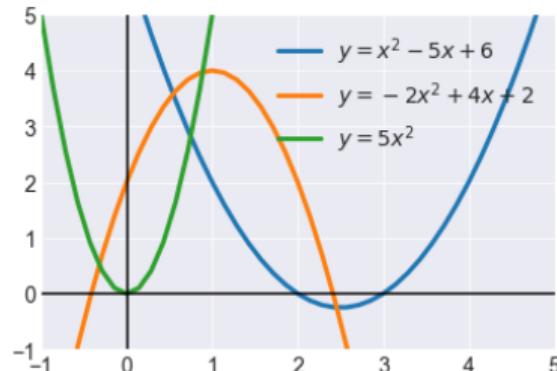
And the formula for a quadratic:

$$y = ax^2 + bx + c$$

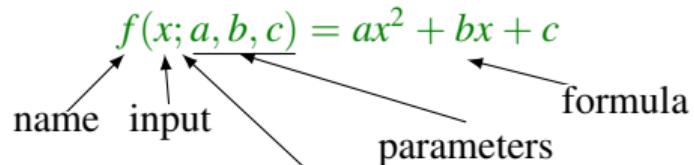
with given coefficients  $a \neq 0$ ,  $b$  and  $c$ .

Examples include

$$y = x^2 - 5x + 6, \quad y = -2x^2 + 4x + 2, \quad y = 5x^2$$



Now consider the collection of all possible quadratics — this gives us the **family of quadratic functions**, i.e., all functions of the form



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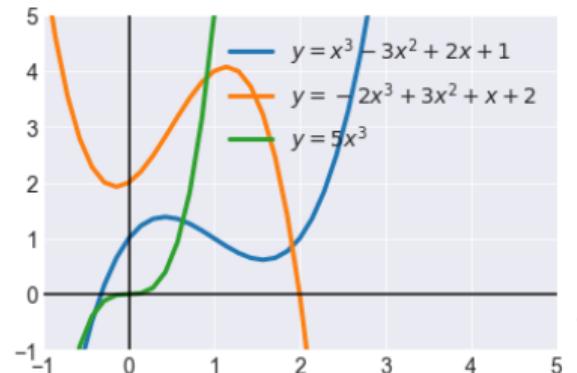
And the formula for a cubics:

$$y = a_3x^3 + a_2x^2 + a_1x + a_0$$

with given coefficients  $a_3 \neq 0$ ,  $a_2$ ,  $a_1$  and  $a_0$ .

Examples include

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Now consider the collection of all possible cubics — this gives us the **family of cubics functions**, i.e., all functions of the form

$$f(x; a_3, a_2, a_1, a_0) = a_3x^3 + a_2x^2 + a_1x + a_0$$

We could continue this to quartics (power of 4), quintics (power of 5), sextics (power of 6), ... or we could think about a bigger family — the family of polynomials.

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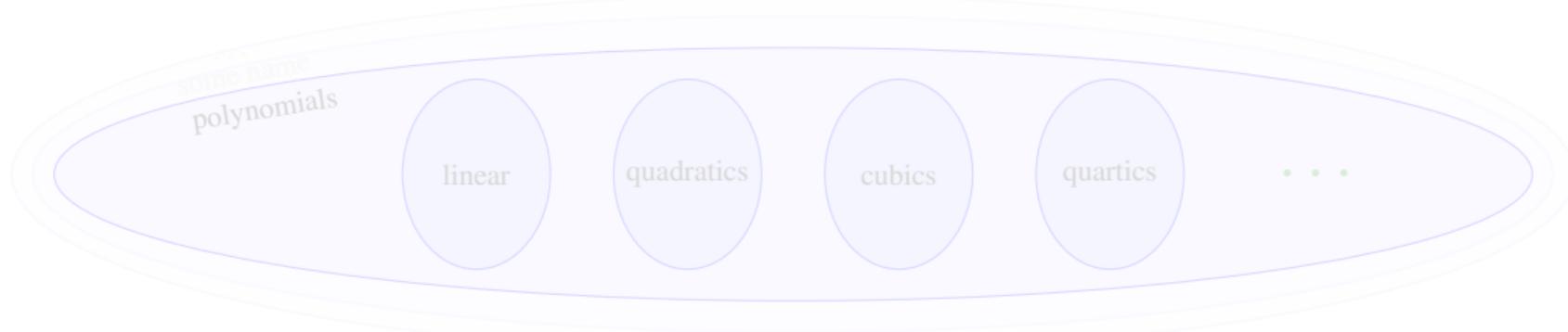
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with vector  $\theta = [a_d, a_{d-1}, \dots, a_1, a_0]$ .

remember we use bold font to indicate vectors.

So we end up with this idea of (nested) families (or **sets**) of functions



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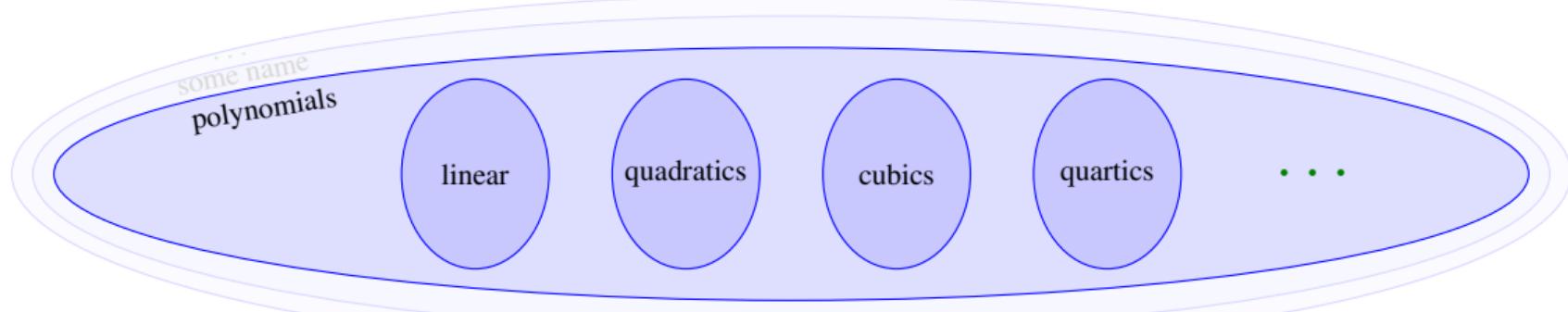
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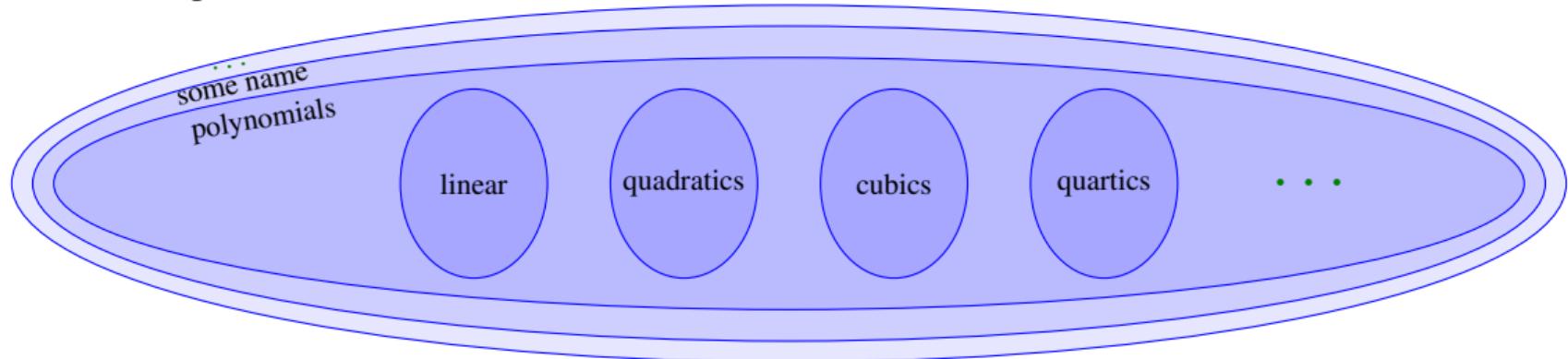
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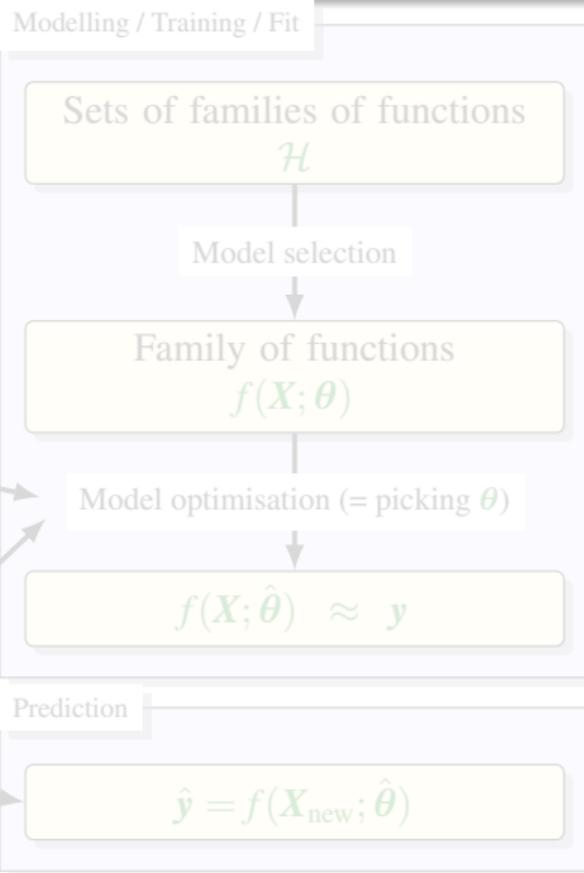
# The ML Problem

- Use hat (^) to indicate predictions.
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Historical Data  
 $X, y$

Cost Function  
 $J(X, y; \theta)$

New Data  
 $X_{\text{new}}$



## Ingredients

- Historical, labeled data
- Unseen, unlabelled data
- Sets of families of functions

## Recipe

- Select a family of functions from all possible families.
- Each member of this family is uniquely determined by its parameter values. Finding the best member (function) is equivalent to finding the corresponding parameter values.
- Using a cost function (which is a measure of the difference between generated labels and given labels) we determine our optimal parameters.
- Finally using best member (function) we can generate predictions for new, unlabelled data.

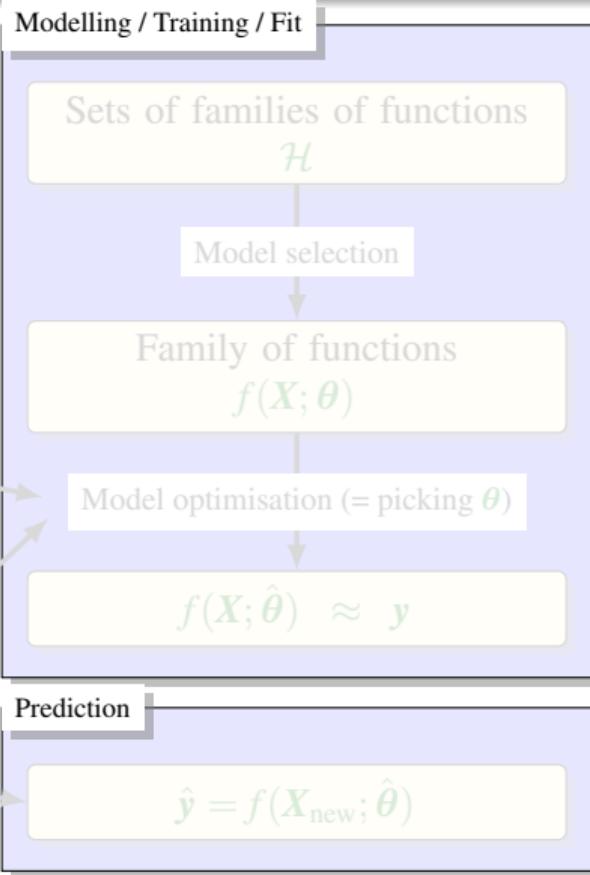
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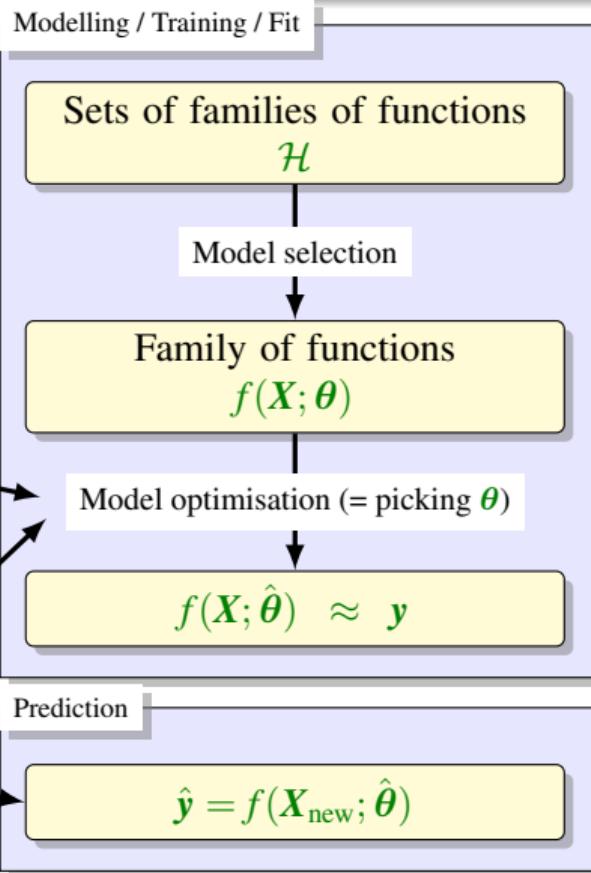
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- Cost is a weighted sum/average over (all) cases/rows/observations.
- In each case/row/observation,  $i$ , want to measure the difference between predicted label,  $\hat{y}^{(i)}$ , and given label,  $y^{(i)}$ .
  - Simplest options are based on the difference — so we have

$$\text{cost}^{(i)} = \left| \hat{y}^{(i)} - y^{(i)} \right| \quad \text{or} \quad \text{cost}^{(i)} = \left( \hat{y}^{(i)} - y^{(i)} \right)^2$$

Absolute value  $||$  or squaring is used to make sure negative and positive costs don't cancel out.

- So a possible cost function,  $J(\mathbf{X}, \mathbf{y}; \boldsymbol{\theta})$  is

$$J(\mathbf{X}, \mathbf{y}; \boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^m \left( \hat{y}^{(i)} - y^{(i)} \right)^2 \quad (\text{MSE})$$

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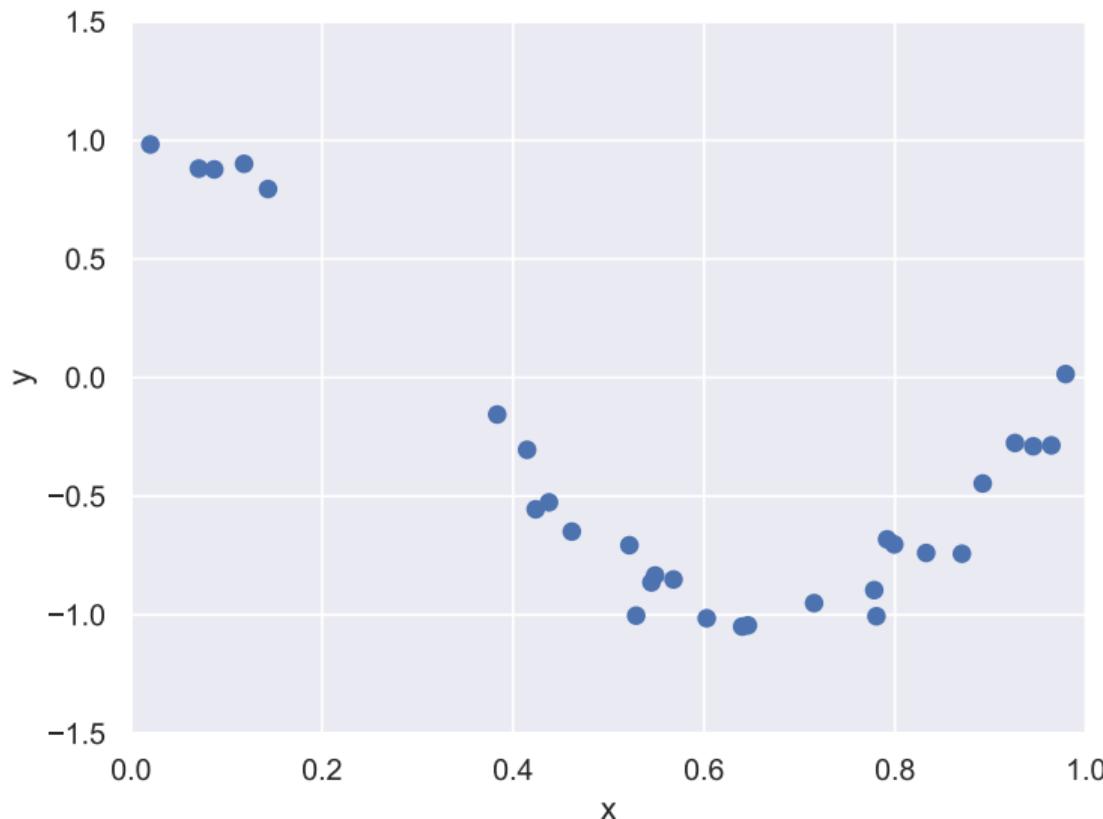
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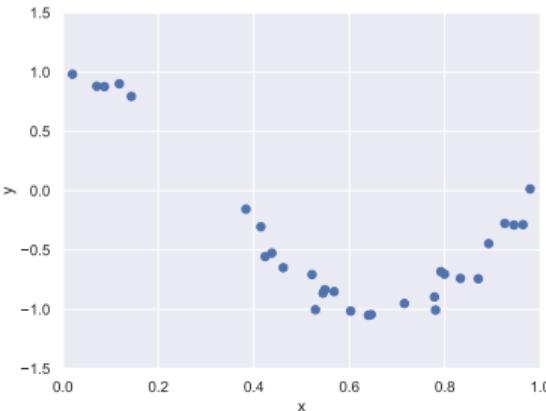
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- Number of parameters is not fixed so have a **non-parametric** method.

- However the order parameter is fundamentally different from the coefficients parameters in the impact a change in its value has (consider switching from line ( $d = 1$ ) to quadratic ( $d = 2$ ) to cubic ( $d = 3$ ), etc.).
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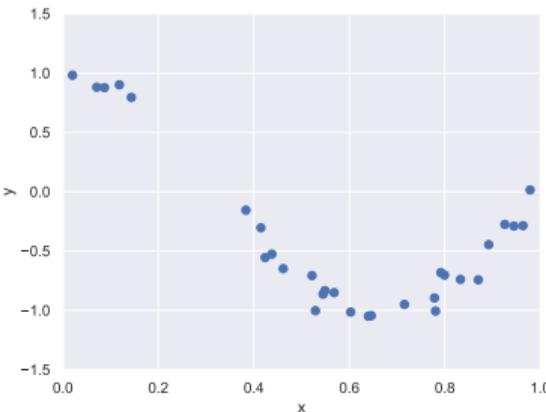
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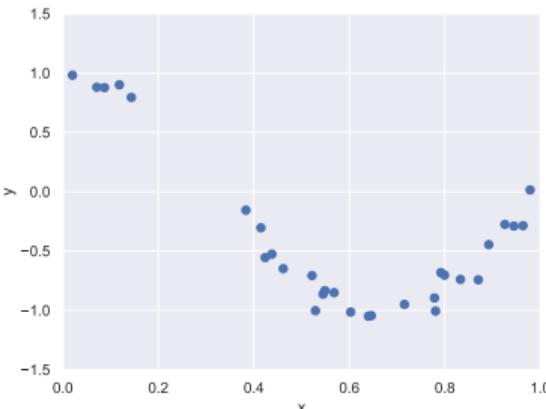
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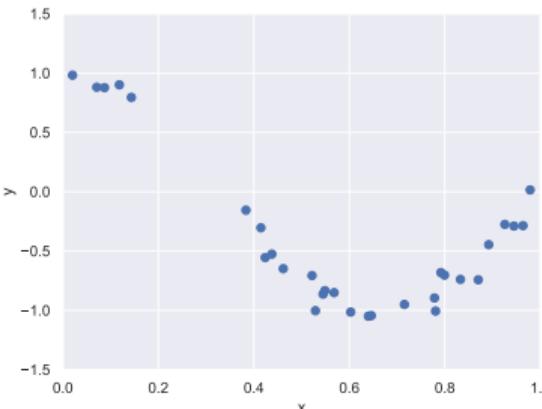
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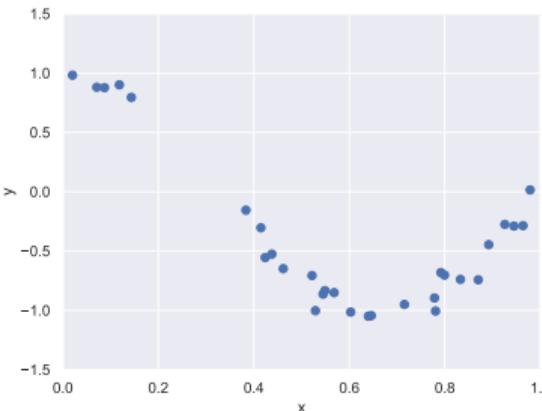
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Given data and a parameterised function, curve fitting is the problem of determining function parameters so that the function output matches desired output as closely as possible.

model

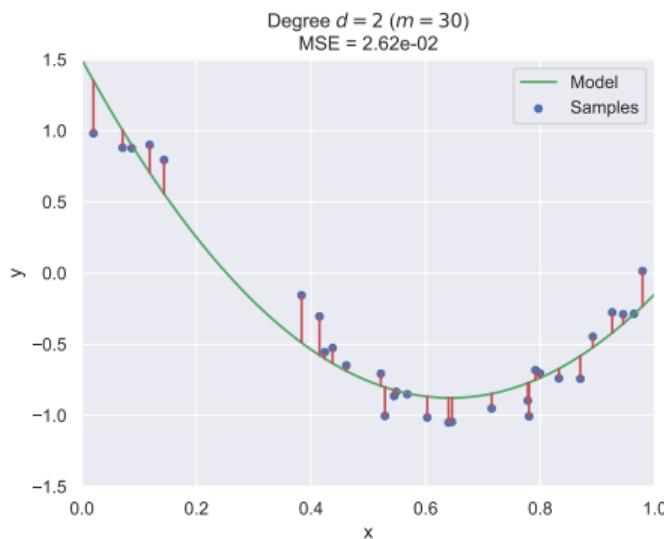
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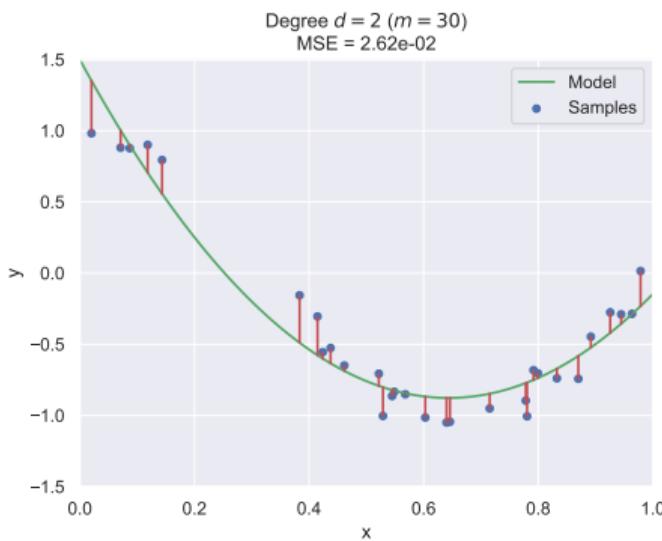
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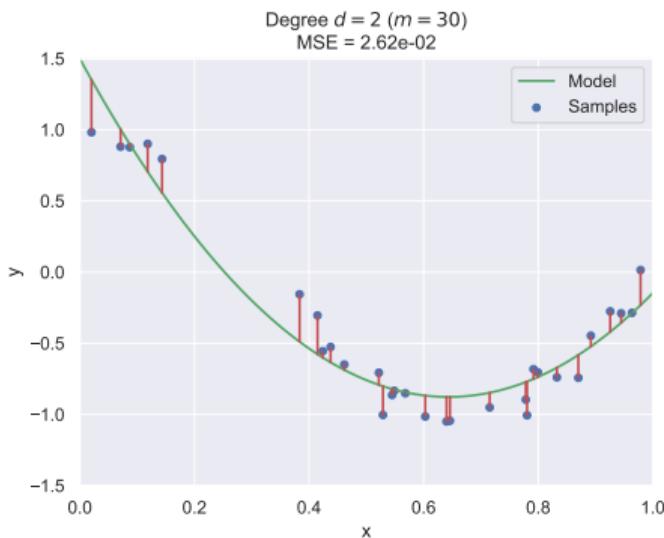
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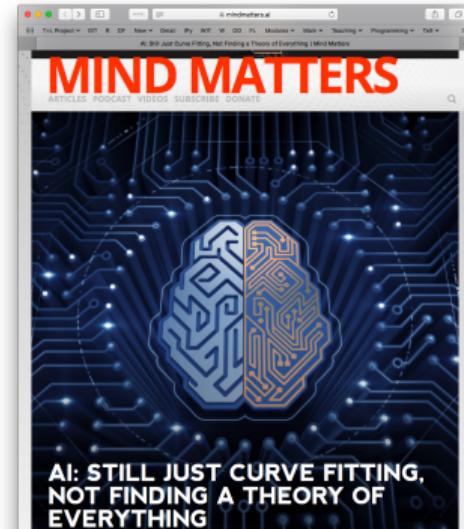
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BY GARY SMITH ON DECEMBER 1, 2020

Judea Pearl, a winner of the Turing Award (the "Nobel Prize of computing"), has argued that, "All the impressive achievements of deep learning amount to just curve fitting." Finding patterns in data may be useful but it is not real intelligence.

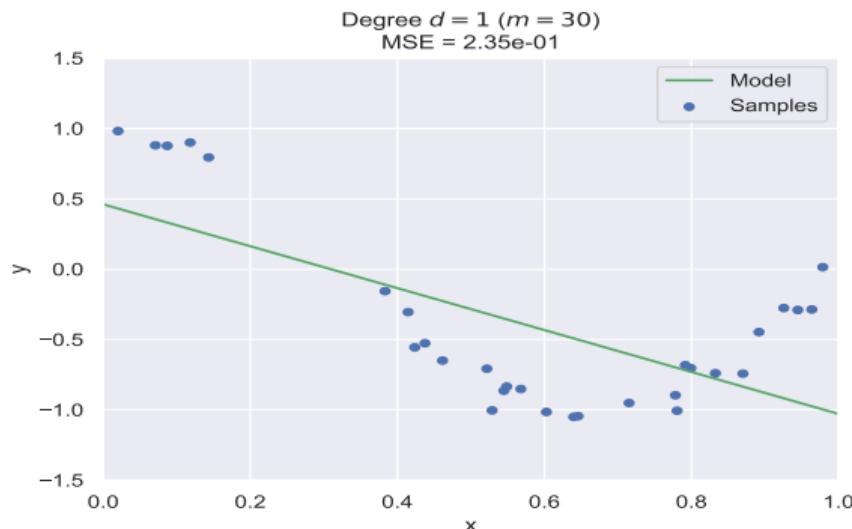
A recent New York Times article, "Can a Computer Devise a Theory of Everything?" suggested that Pearl is wrong because computer algorithms have moved beyond

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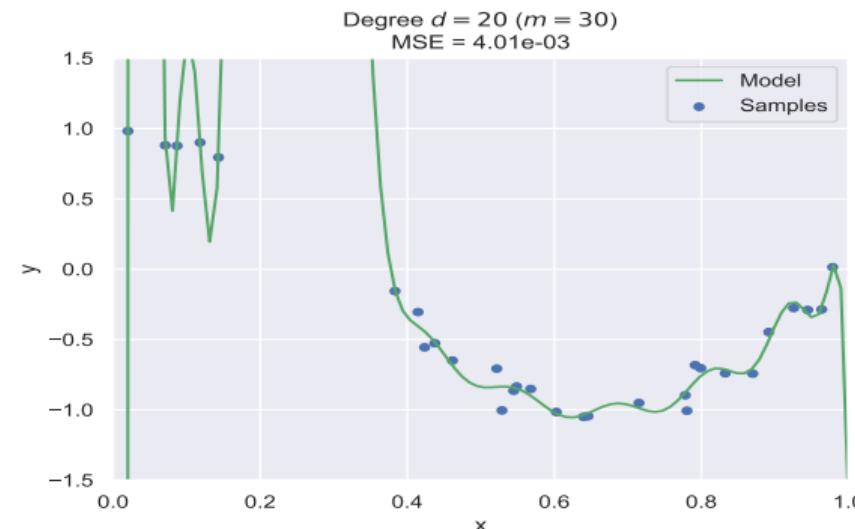
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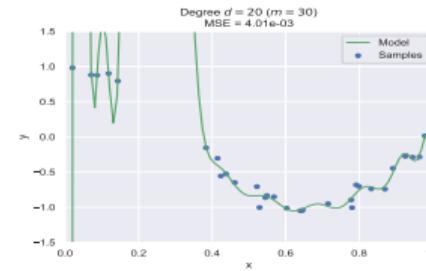
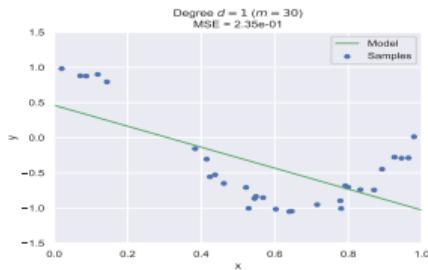
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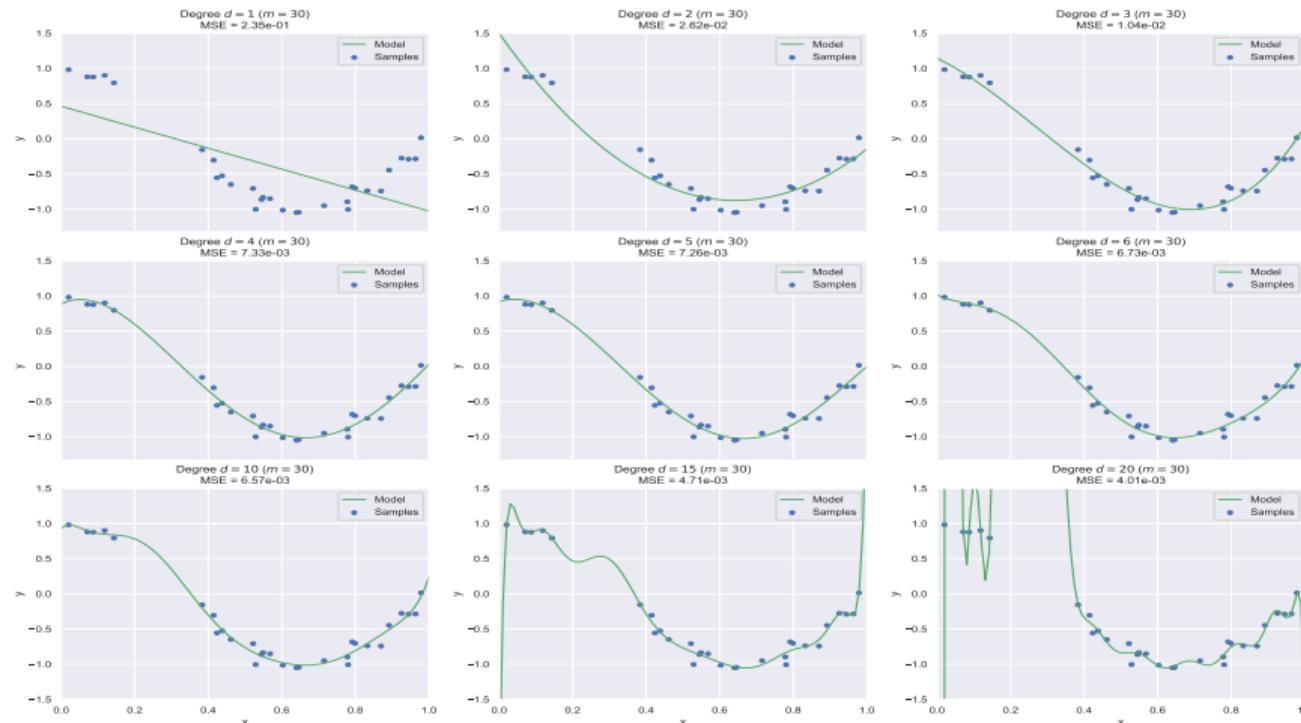
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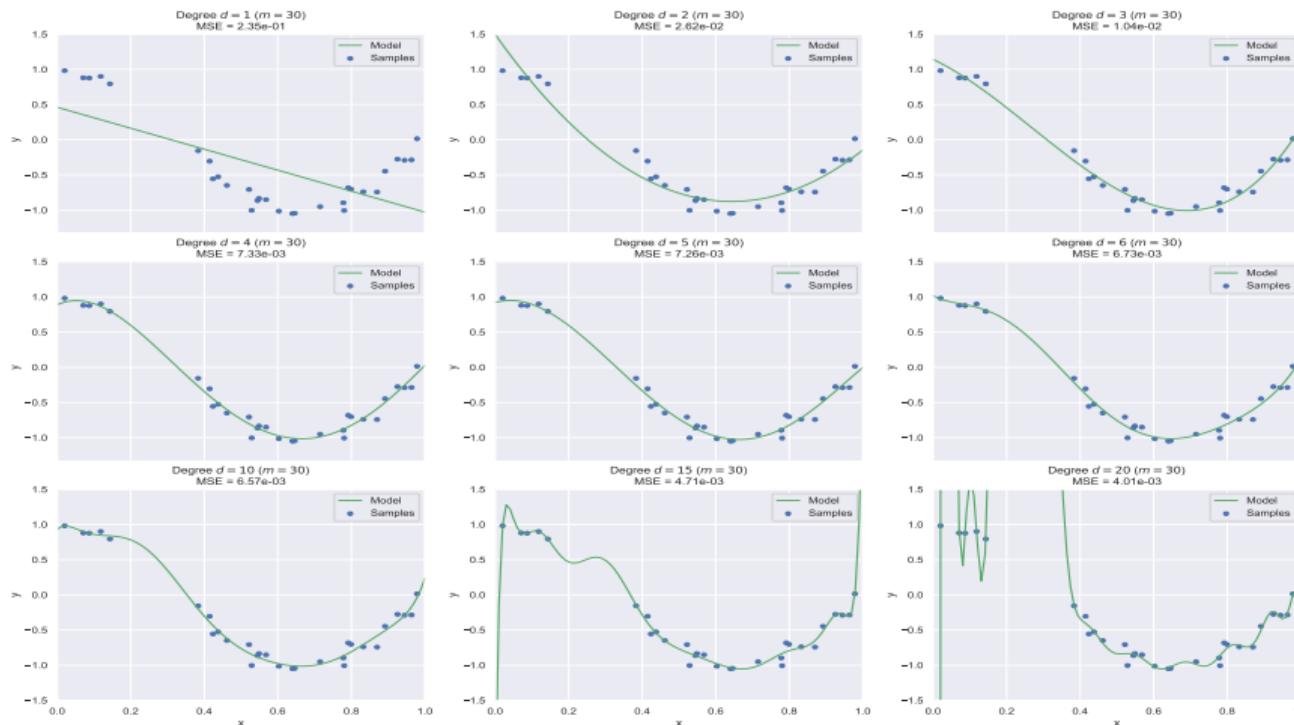
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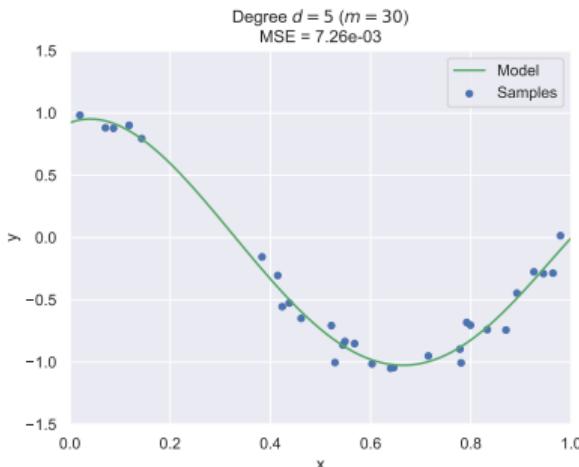
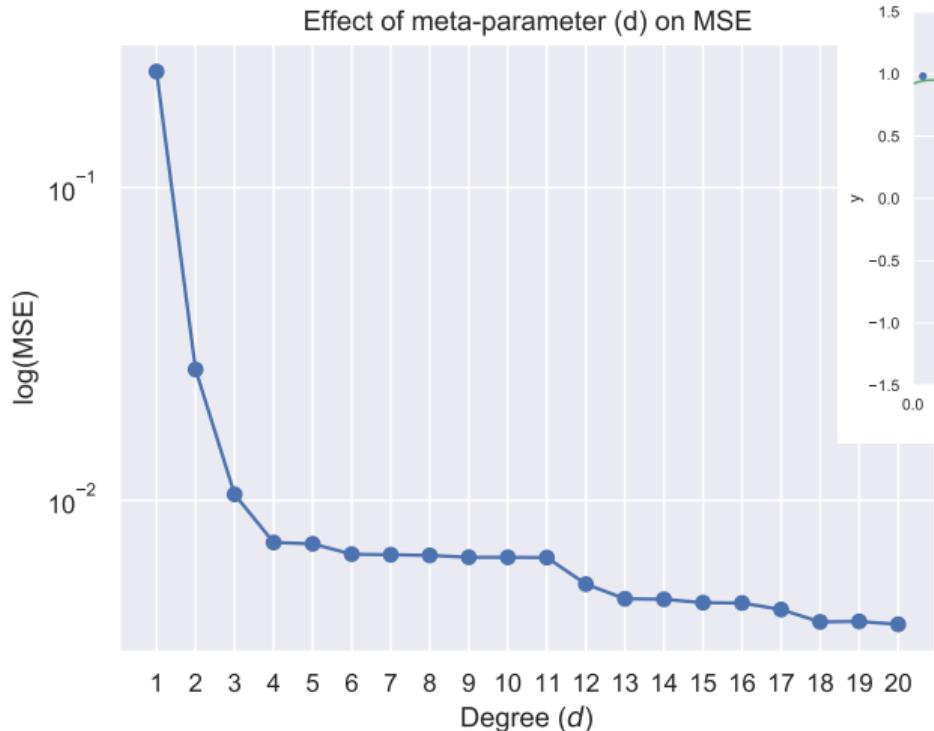


- Degree less than 3 are under-fitting, degree 10 and higher are over-fitting.
- What **objective** metric can we use to determine  $k$ ? (**objective**  $\approx$  automatic)
- Using the Mean Square Error (MSE) appears no good, it is decreasing as we increase the order.

$$MSE = \frac{1}{m} \sum (\hat{y} - y)^2$$

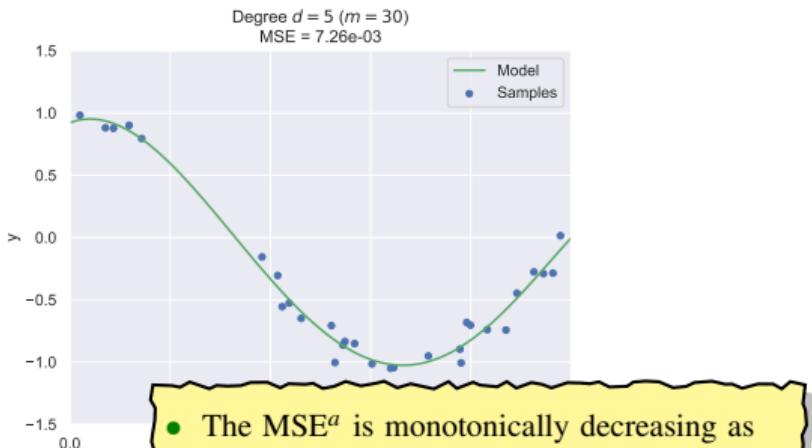
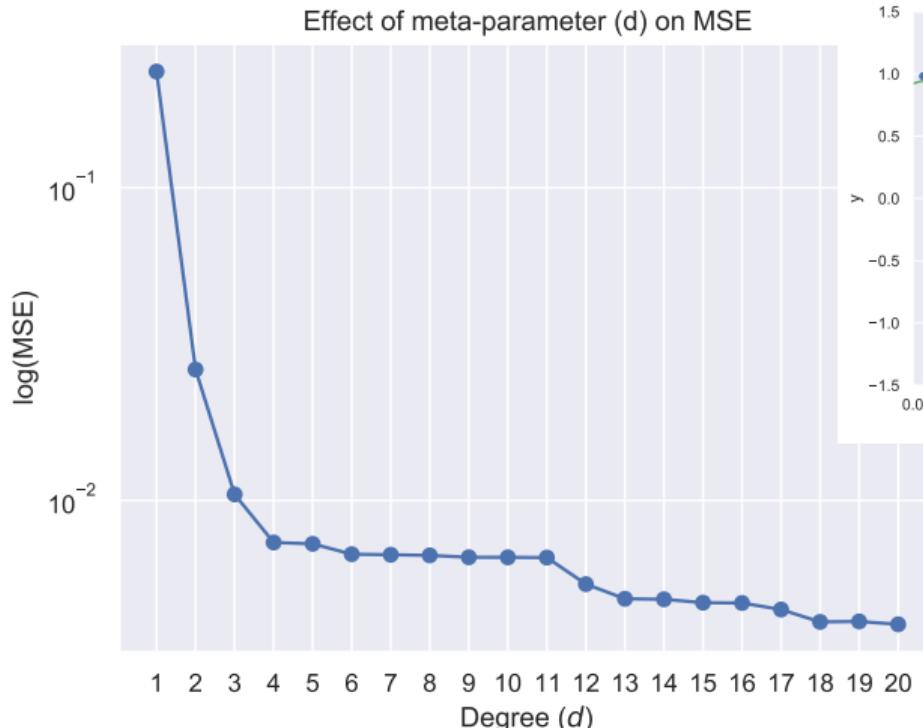
# Effect of Meta-parameter, $d$ , on MSE

Using a for loop over  $d = 1, 2, \dots$  fit model and compute the error (MSE). Plot graph of error against degree,  $d$ :



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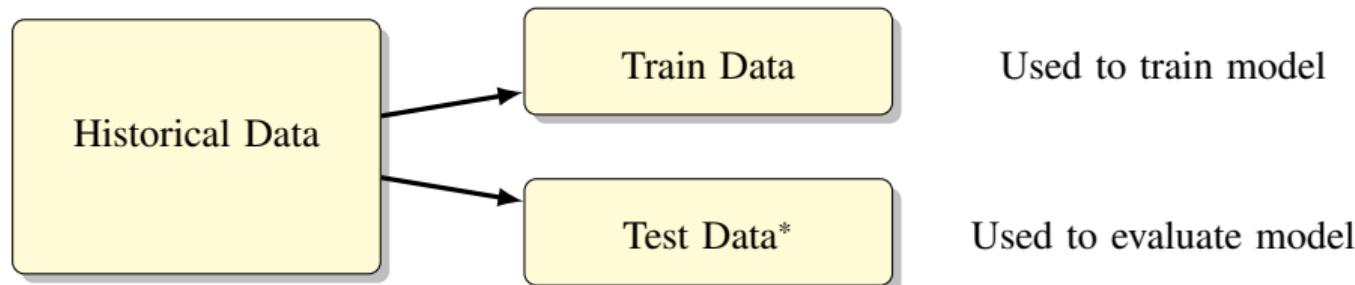


- The MSE<sup>a</sup> is monotonically decreasing as the polynomial order increases.
- Can only estimate the optimal value for  $d$  (about 5) by looking at plots of the fit — subjective, computationally prohibitive and not scalable.

<sup>a</sup>Note we use logarithmic scale when plotting values over relatively large scales

# Splitting Historical Data into Train and Test Data

The issue is not with the MSE metric, but how we have used it.

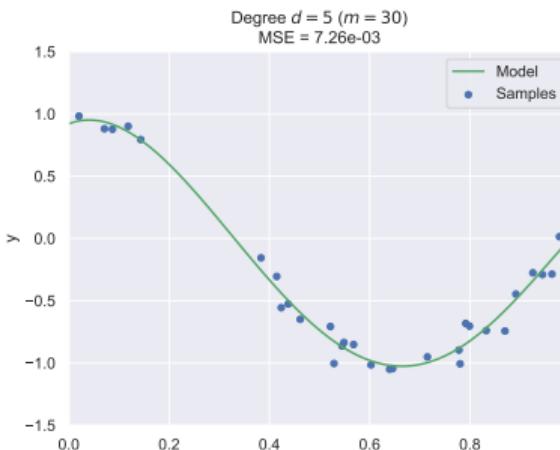
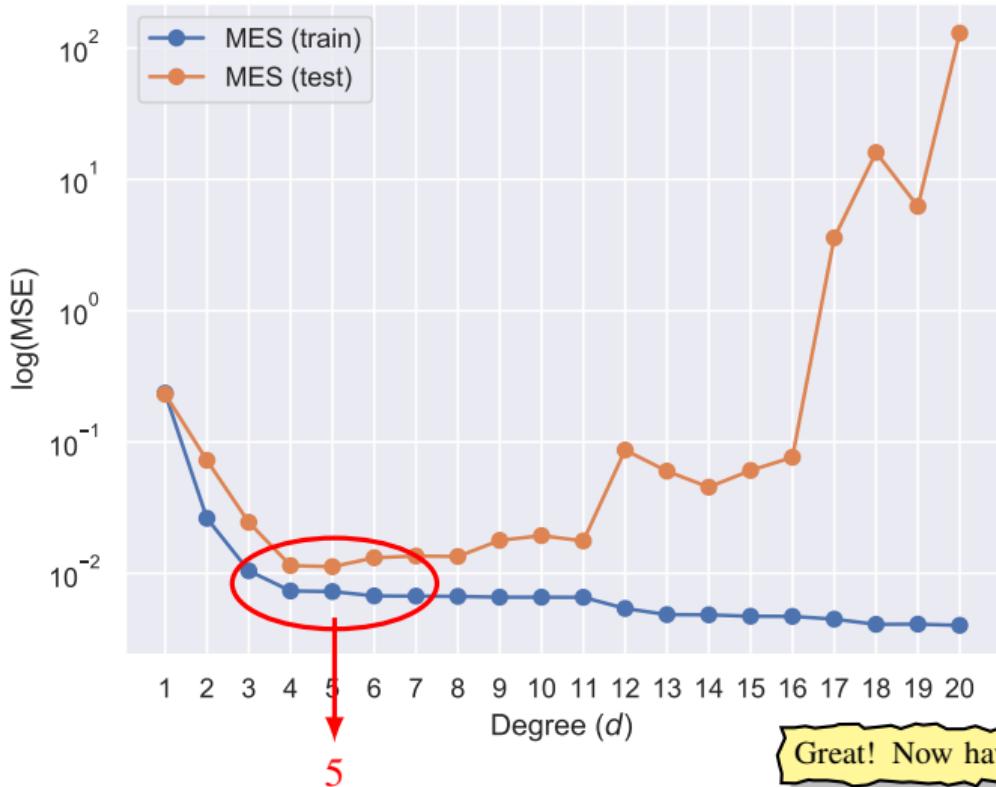


- Using the training data for both model fitting and evaluation purposes can lead to overly optimistic estimates about the performance of the model.
- This can result in choosing a suboptimal model that performs poorly when predicting on new data.
- Now my issues are
  - “How do we split the historical data?”* Default to train/test split of say, 60%/40%.
  - “What happens if I don’t have enough data?”* Use cross-validation (CV) methods.

\*The label ‘test’ is problematic because this is often split again into ‘test’ and ‘validation’. Some practitioners, eg Andrew Ng, use the term ‘dev’ set instead.

# Effect of Meta-parameter on MSE (train and test data)

Effect of meta-parameter ( $d$ ) on MSE



- Method: Fit the model to the train data and then evaluate it on the previously unseen test data.
- Select value of meta-parameter based on MSE (test).

Great! Now have a objective / automatic method

# Bias and Variance

Under-fitting/over-fitting can be thought of in terms of high-bias/high-variance:

## ➤ Bias

The error due to the difference between the expected (or average) prediction of our model and the correct value which we are trying to predict, over different realisations of the model.

Under-fitting results in high-bias

## ➤ Variance

The error due to variance is taken as the variability of a model prediction for a given data point between **different realisations** of the model.

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The different realisations of the model can be computed by repeating the model building process over multiple datasets, or by sampling the given dataset.

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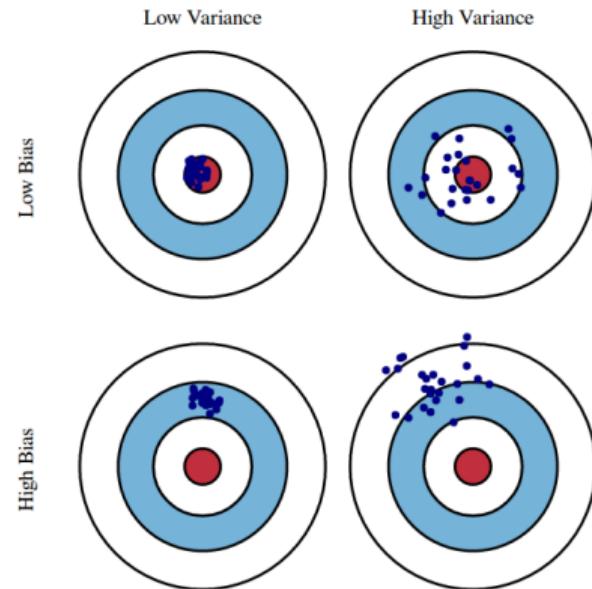
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—Scott Foremann-Roe, June 2012

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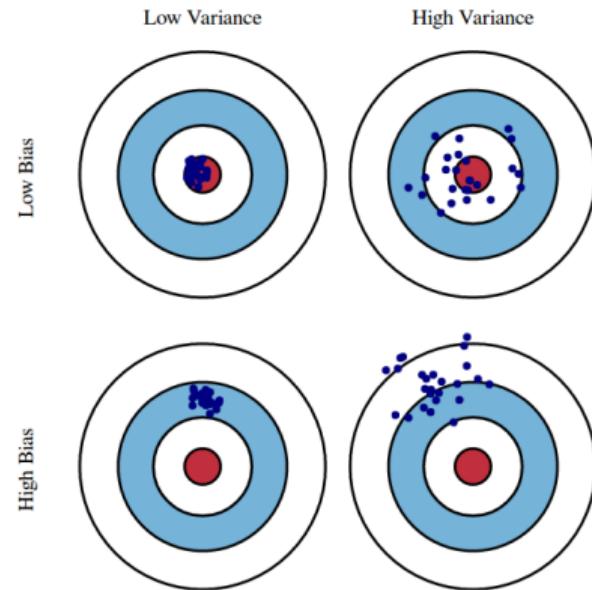
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Over-fitting results in high-variance

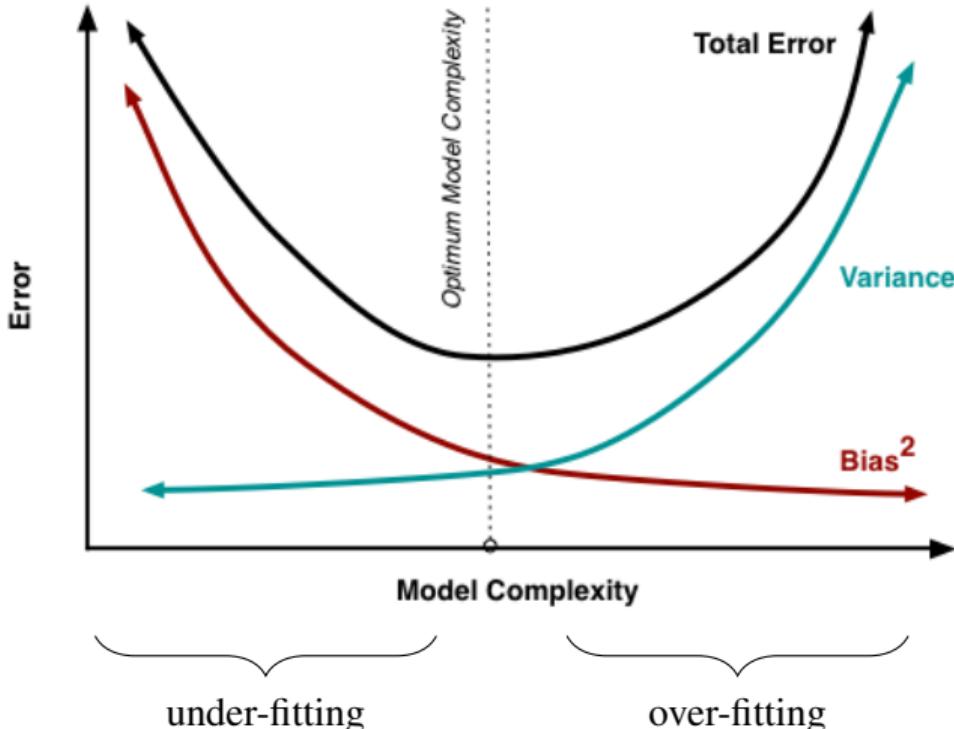
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# Bias–Variance Tradeoff

$$\text{Error} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

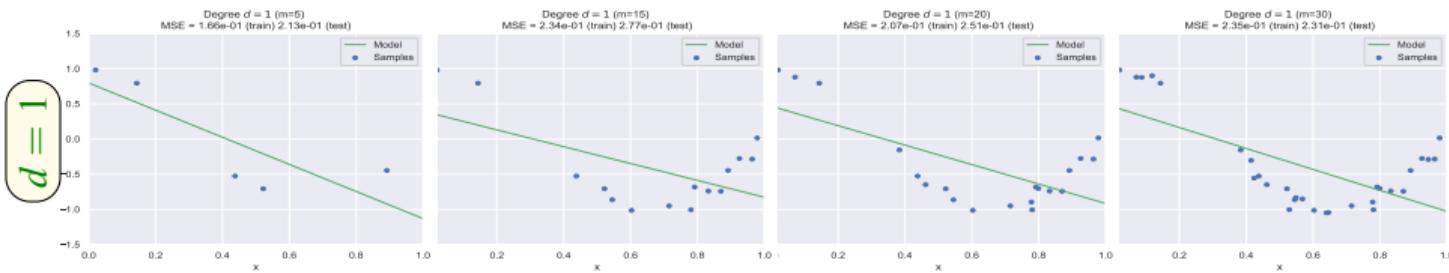


# Effect of Number of Observations and Over/Under-fitting

**Question:** How does the best fit model change as,  $m$ , the number of observations change? ...

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- When under-fitting (high-bias) the model is not sensitive (can't represent) to changes in the data.
- When over-fitting (high-variance) the model is too sensitive to changes in the data.
- More data does not affect an appropriate model much.

More data helps to reduce effects of overfitting.

$m = 5$

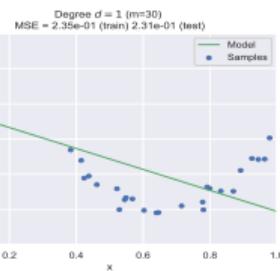
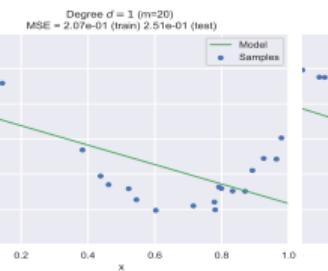
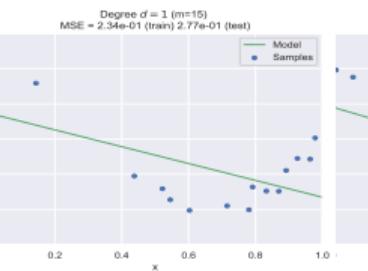
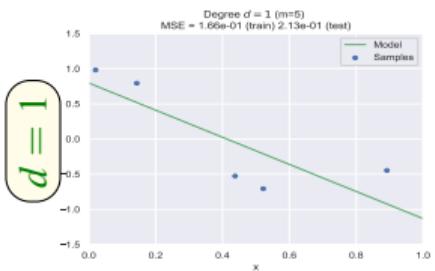
$m = 15$

$m = 20$

$m = 30$

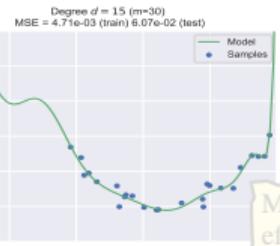
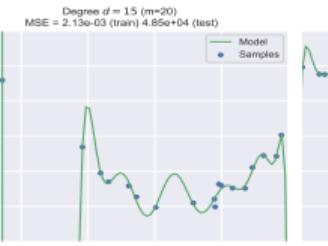
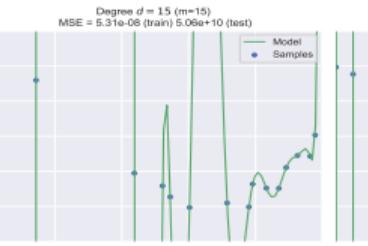
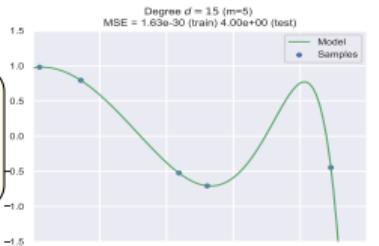
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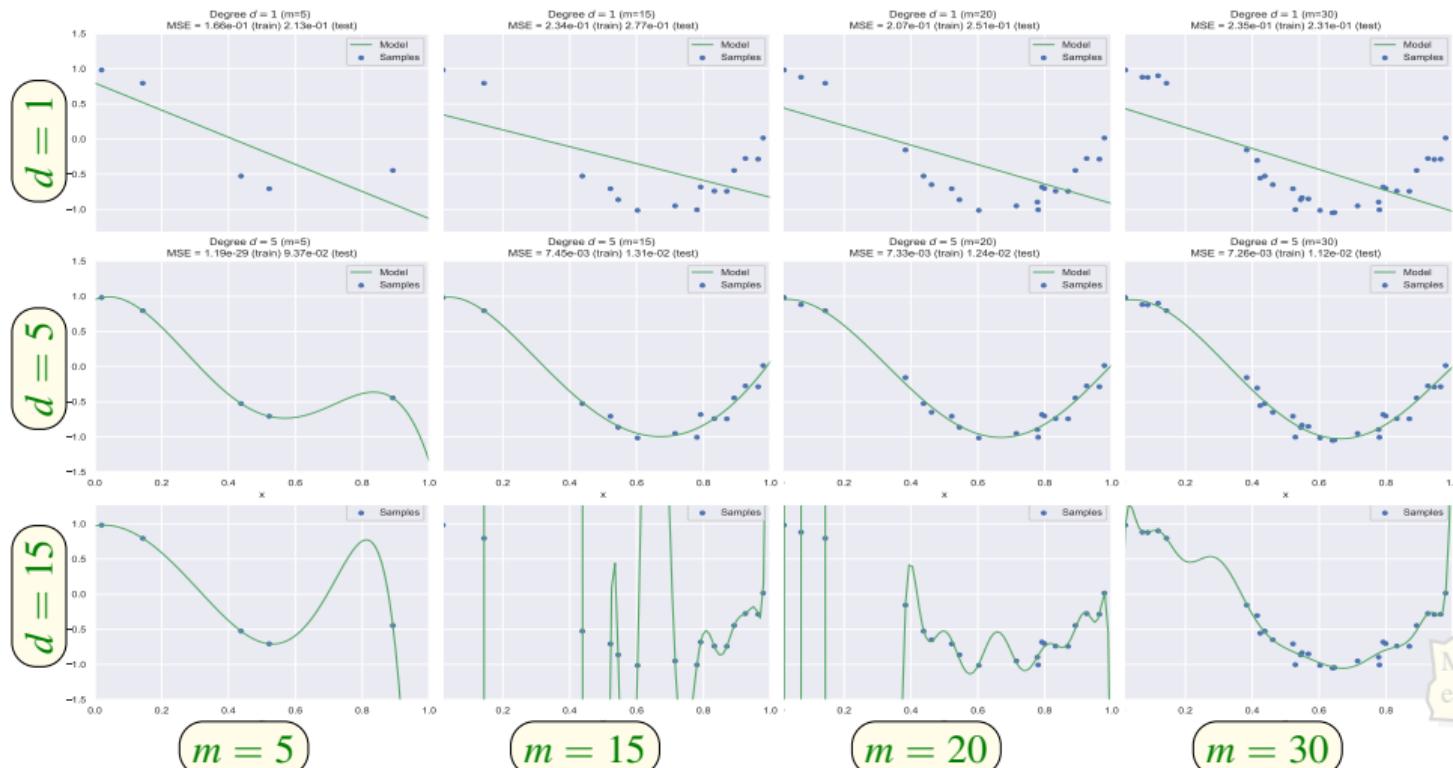
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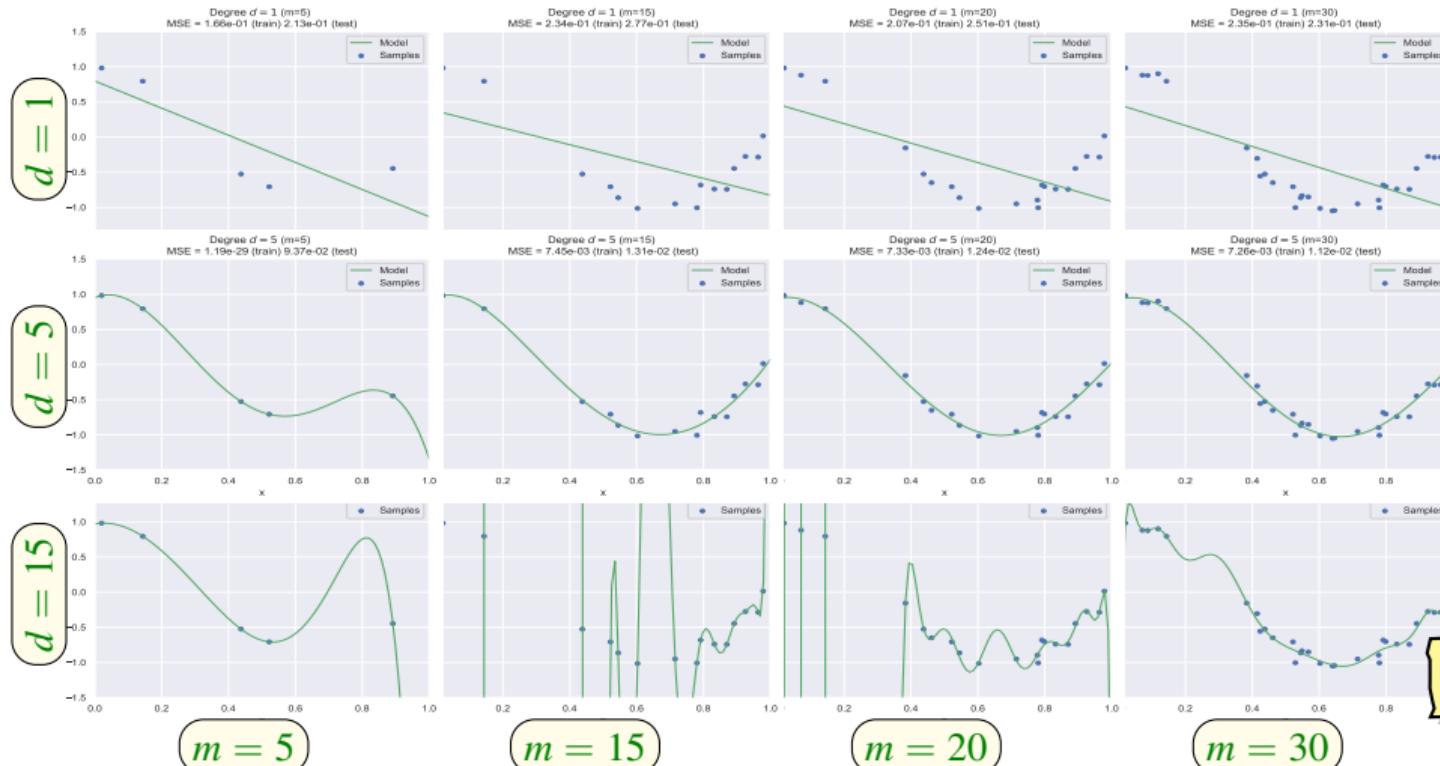
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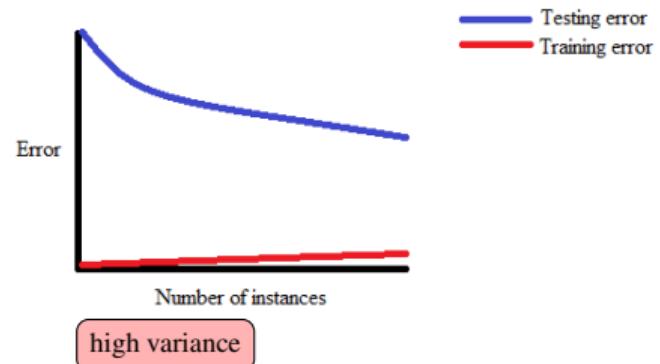
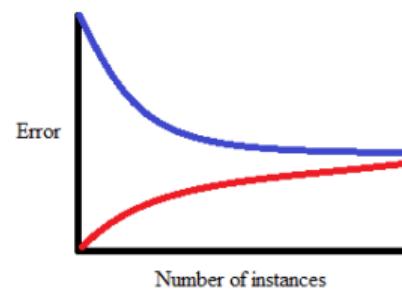
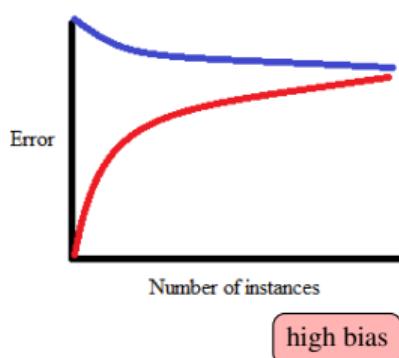
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# Learning Curves

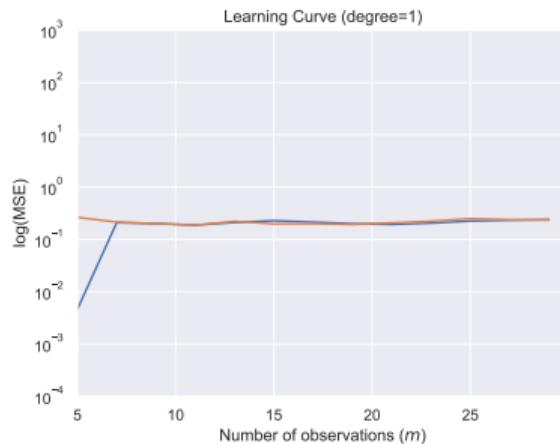
- The **learning curve** is a graph that compares the performance of a model on training and testing data over a varying number of training instances
- Should generally see performance improve as the number of training points increases.
- The comparison of performance on training and testing datasets is an indicator of how well the model can generalise to new data.
- Learning curve allows us to verify when a model has learned as much as it can about the data:
  - The performances on the training and testing sets reach a plateau.
  - There is a consistent gap between the two error rates.

## Idealised Learning Curves

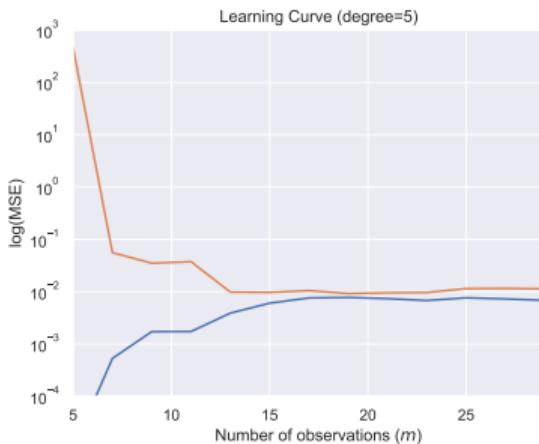


# Practical Learning Curves

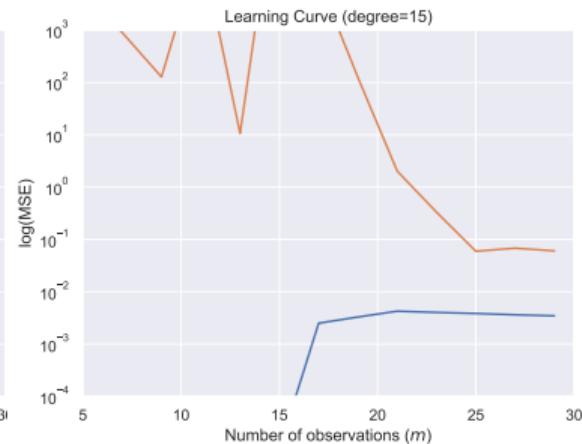
Real learning curves are more noisy, but the general structure is still visible — for our generated data set we have



high bias



high variance



## Resolving High Bias/Variance

- High-Bias — Increase model complexity
- High-Variance — Decrease model complexity or/and increase number of observations.

# Overview of Testing and Validating a Model

No single approach works, so need mixture of

- **theoretical** — various measures of statistical validity to determine whether there are problems in the data or in the model
  - Test for normality, uniform variance, ...
- **practical** — separate the data into train and test sets and evaluate on test (or validation set).
  - **accuracy** — how often/close does the model match the target?
    - Which metric should be used?
  - **reliability** — how robust is the model to different train sets?
    - How much data is needed for convergence (training)?
  - **utility** — can the model be used in practice? what is the marginal benefit of using the model?  
Metrics **lift** and **gain**: the improvement that you get from using a data mining model, when you compare it to random guessing (or other model).
- **reality check** – area experts to review model.

# Cross Validation Methods

Splitting the dataset into train and test data results in another source of variation, especially for small datasets. Methods that address this:

## Holdout Method

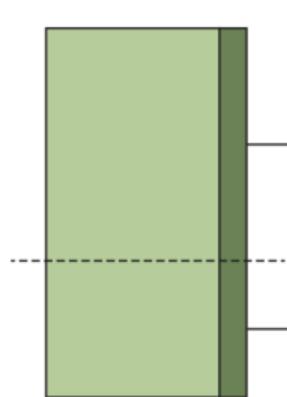
- Simplest method — just select a train/test split ratio and randomly allocate observations to train and test datasets.
- The optimal parameters from training and the error estimates on the test dataset can be noisy.

## K-Fold Cross Validation

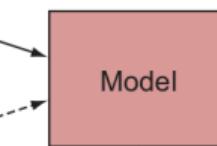
- Split the dataset into  $k$  disjoint subsets, called folds (typical choices for  $k$  are 5, 10, or 20).
- For each fold, a model is trained on all the data except the data from that fold and is subsequently used to generate predictions for the data from that fold.
- After all  $k$ -folds are cycled through, the predictions for each fold are aggregated and compared to the true target variable to assess accuracy.
- This results in noise estimate for the parameters and the error but is more computationally intensive approach than the holdout method.

# Holdout Method

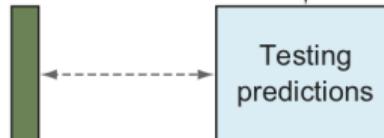
1. Randomly split training instances into training and testing subsets



2. Train an ML model on the training subset



3. Make predictions on testing subset

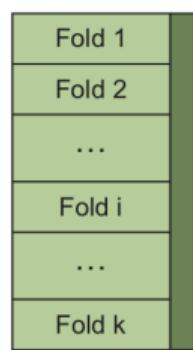


Legend:  
■ Features  
■ Target

4. Comparing testing predictions to testing target to assess accuracy

# K-Fold Cross Validation

1. Randomly split training instances into  $k$  equal-sized subsets



For  $i$  in  $1:k$



2. Train an ML model on the training subset

Model

Ignore target when predicting

3. Make predictions on fold  $i$  subset

Fold  $i$  predictions

■ Features  
■ Target

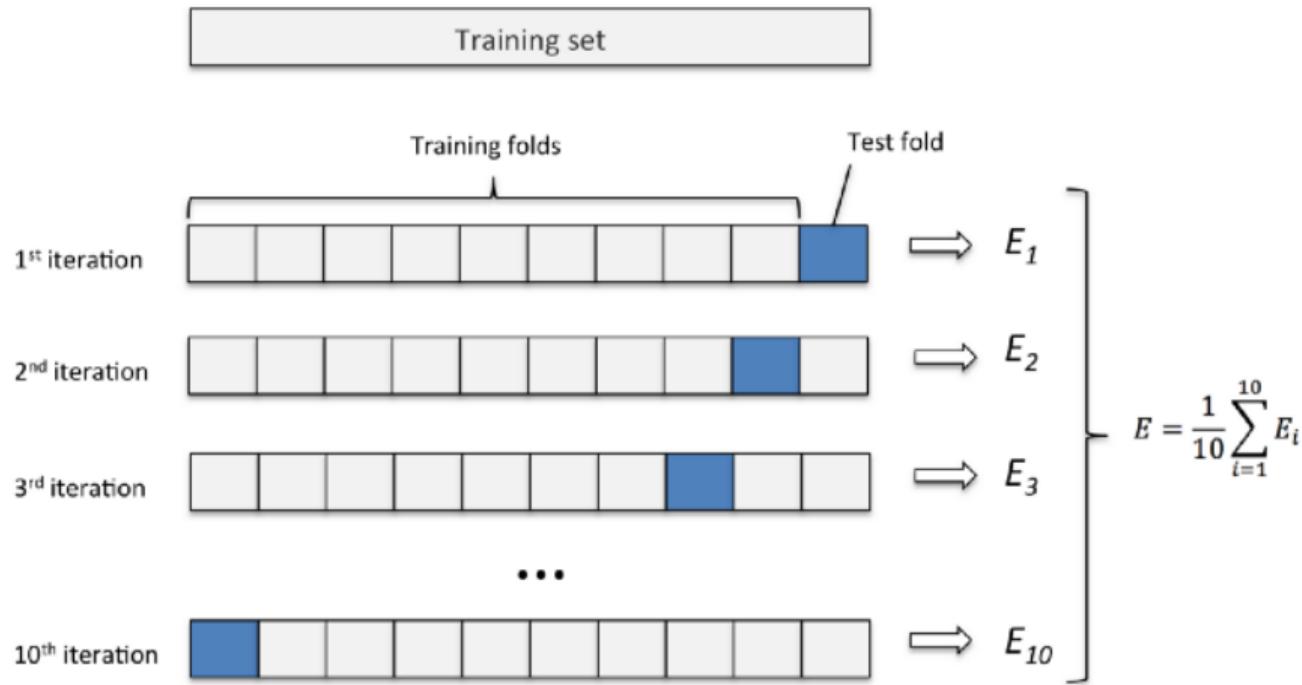
5. Compare CV predictions to target to assess accuracy

4. Store fold  $i$  predictions in the CV predictions array

CV predictions

# K-Fold Cross Validation

Typical process: Train model  $k$  times to generate  $k$  estimates of model performance and then average.

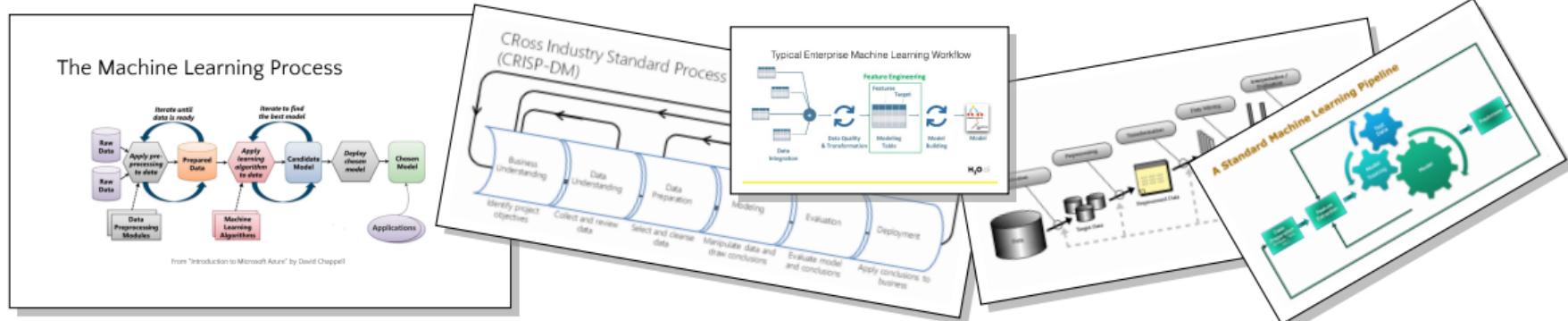


# Outline

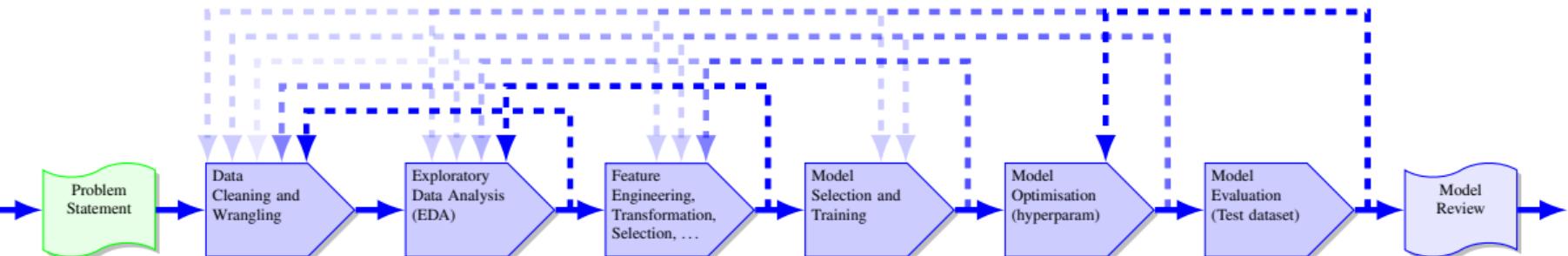
1. Machine Learning (ML) Overview	3
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1.2. Taxonomy of Machine Learning Methods	8
1.3. Statistical Models vs Machine Learning Models	10
2. Notation	11
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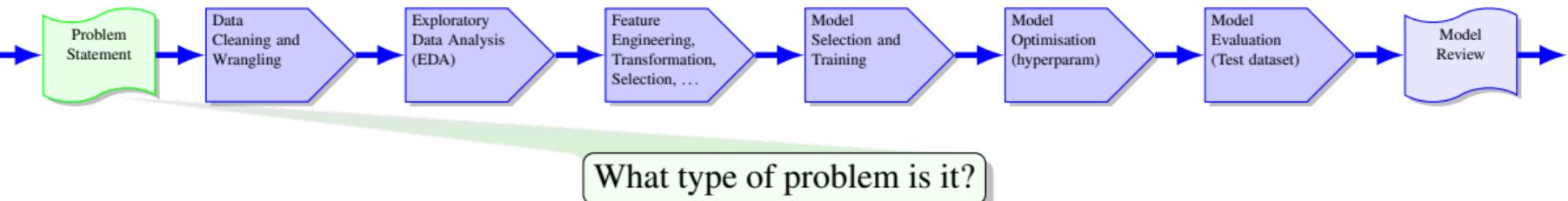
# Data Mining Workflow

There are many, many ...

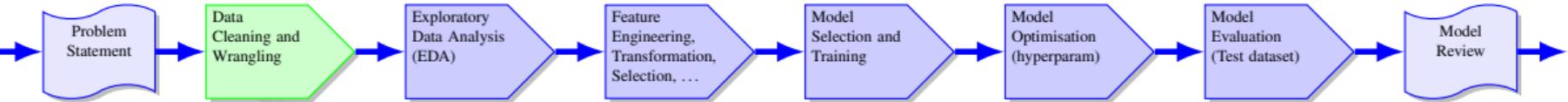


So why not make YADMW (Yet Another Data Mining Workflow)?





- Exploratory data analysis  
Do we just want to see what the data says?
- Association / Rule finding  
Are we searching for relations/patterns?
- Hypothesis testing (Statistical)  
Do we have a theory we wish to test?
- Model building  
Do we wish to build a representation of some pattern within the data?
  - **Supervised** ⇔ data split into input variables (**features**) and output variable(s) (**target(s)**)
    - **Classification** (target is **categorical**) vs **regression** (target is **continuous**)
  - **Unsupervised** ⇔ no target
    - **Clustering** — grouping similar cases



How to import and prepare data for subsequent analysis/processing?

- Multiple file formats
  - Pandas supports a wide collection of file formats but default options often need to be changed to suit data.
  - Main file format (Comma Separated Values ([csv](#))) does not support meta-data, is slow, and results in large files  
⇒ use other formats ([pickle](#), [feather](#)) to store datasets between steps in the workflow.
- Assumptions made by input parser can be important (i.e., bite you when you least expect)
  - Scientists rename [human genes](#) to stop Microsoft Excel from misreading them as dates
  - Pandas vs excel use different heuristics to decide on data type of each variable.
- Sub-tasks
  - Check dimension (number of [rows/cases](#), number of [columns/variables](#)).
  - Check data types ([categorical](#), [ordinal](#), or [numerical \(discrete/continous\)](#)) of each variable.
  - Check for missing values, encoding errors, etc.
  - Merge tables, apply filters, and general data wrangling to generate (tabular) dataset suitable for EDA.



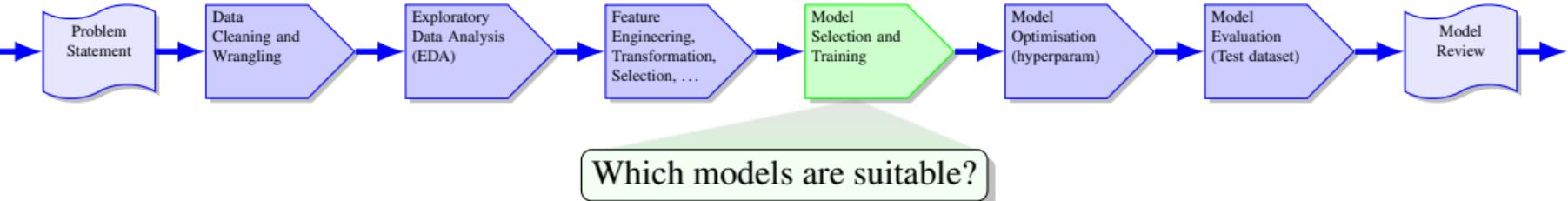
- Univariate descriptive statistics — examine each variable
  - What are typical values?
  - What is the variation / spread / range?
  - What does the data look like ... bell curve, bath tub curve, etc. ?
- Bi- / multi- variable descriptive statistics
  - Identifying relationships between variables.
- All descriptive statistics methods summarise data:
  - ✓ A summary is good since it helps to focus on simpler and important aspects.
  - ✗ A summary is bad if it focuses on irrelevant or the wrong aspects.
  - ⇒ Need to use multiple methods, be aware of their strengths/deficiencies.



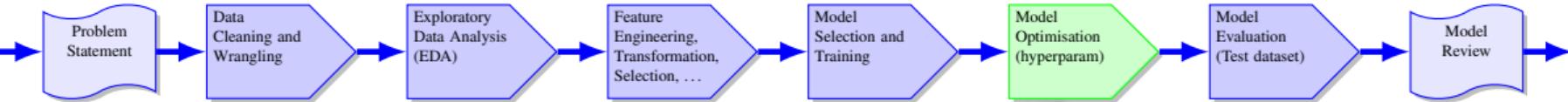


Can we transform, encode/bin, select, . . . , the given features to improve model training?

- Better features can mean:
  - Better model performance and reduce training times.
  - Simpler models become applicable — think linear/logistic regression.
  - More explainable models — the future of machine learning (hopefully).
  - Cheaper and easier models to deploy.
- Feature selection reduces the number of features used in the model:
  - Drop features that have low variability.
  - Drop features that have no relation to target.
  - Drop features that are highly related to other features — **multicollinearity**.
  - Keep features whose addition to model have the largest improvement in model score.
- Feature extraction merges existing features to generate (hopefully) fewer features with essentially all the variation.

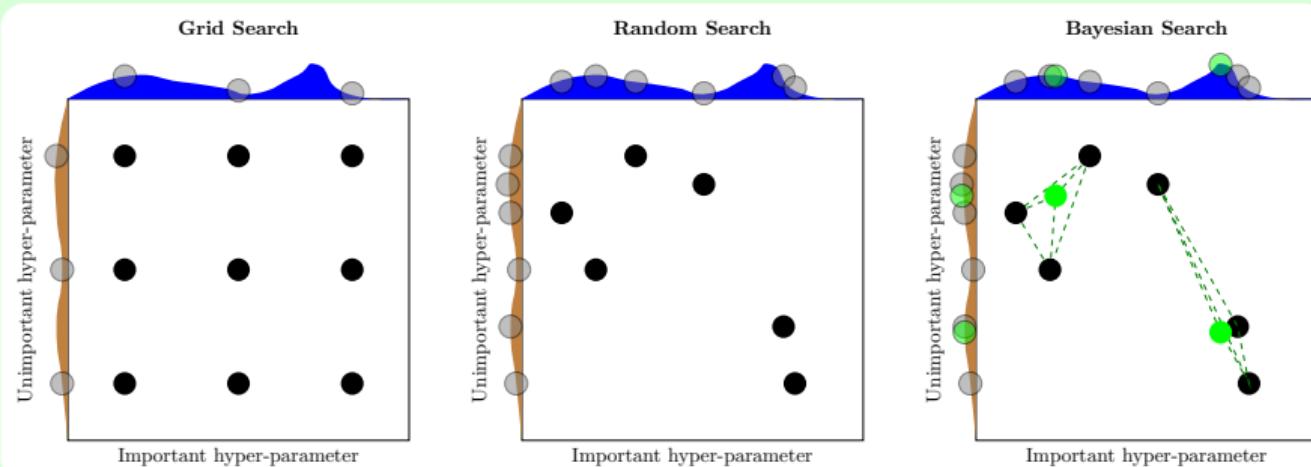


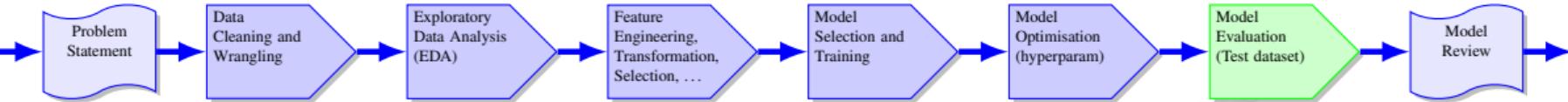
- Models vary greatly in terms of capabilities/deficiencies — usually aim to build a short list of candidate models, which are subsequently optimised in the next step.
- Select models based on different algorithms/approaches.
- Select (loss function and) evaluation metric.
  - **Loss function** is used to train model, **evaluation metric** is used to evaluate model (post training).
- Relative model performance can help identify issues with data.
  - Outliers can negatively affect linear regression but have smaller impact on decision tree based models.



## How do we determine optimal values of the hyper-parameters?

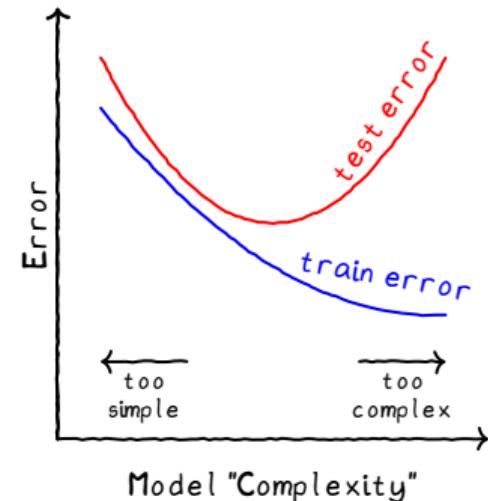
- Most models have options which control how a model “learns” from the training data.
- Three search strategies: Grid search < Random search ≪ Bayesian search

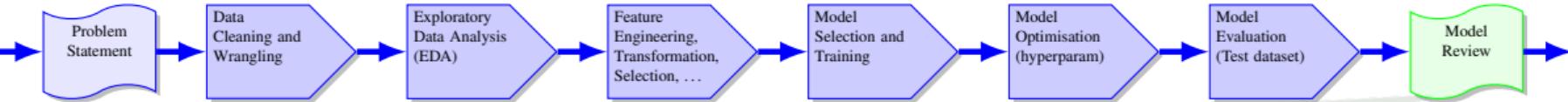




How well does the model generalise (to unseen data)?

- In the machine learning approach (vs statistical approach) we rely on model performance on **unseen data** to evaluate models.
  - Split data into train/test, only use train dataset for all modelling decisions.
  - [Data leakage \(MachineLearningMastery article\)](#), where information outside the train dataset is used in model building.
- Is there evidence for overfitting?
  - Does the model perform much better on training dataset than on the test dataset?
- Multiple techniques to address overfitting:
  - Regularisation (linear / logistic regression).
  - Trimming (decision trees).
  - Dropout (neural networks), Batch normalisation (CNN).





How well have we addressed the problem statement?

- A what level of **accuracy** (or other metrics) does a model become useful?
  - This is a business, medical, ... decision
  - The larger the relative payoff the weaker the model can be and still be useful.
- OK, finally ready to implement/deploy model ...
  - Separate skillset / concerns
  - MLOps = ML + DevOps
  - Monitoring of model drift needed.
- towards data science What is MLOps — Everything You Must Know to Get Started

**Q:** Why don't we automate all of this sh\*tstuff?  
Tools are getting better and easier to use, but need intervention/direction (data can be weird in weird ways)



- [xkcd.com/2054](http://xkcd.com/2054)