Machine Learning For Design

Lecture 8 - Designing And Develop Machine Learning Models / Part 2

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23/03/2022

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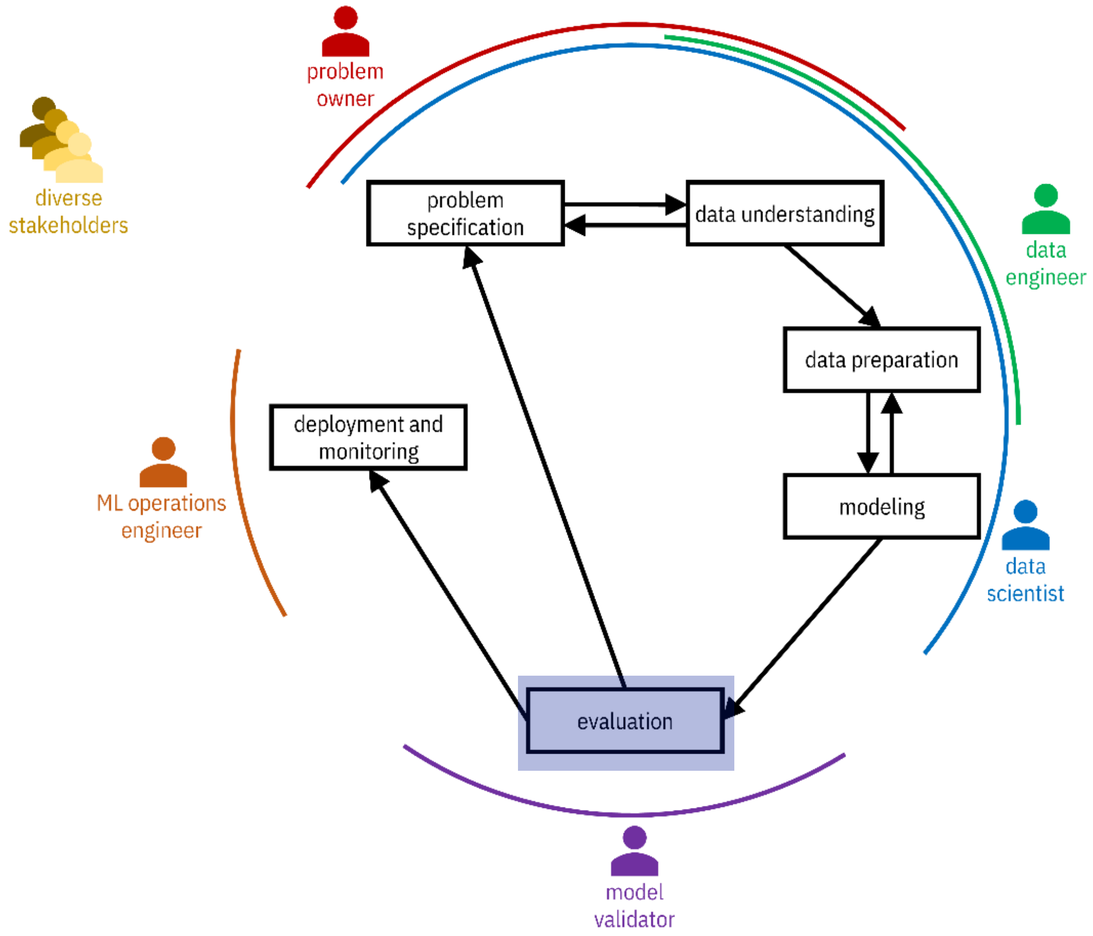
Evaluation

Cross-Industry Standard Process for Data Mining (CRISP-DM) methodology

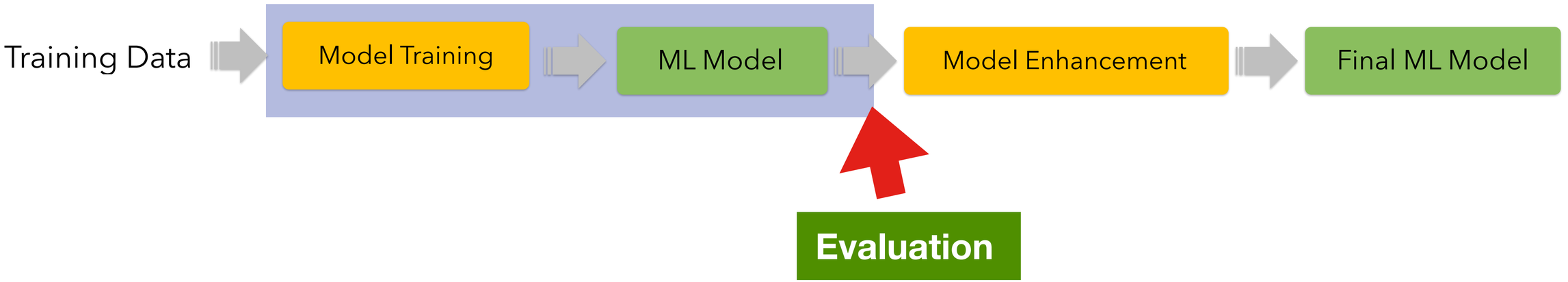
Lecture 2



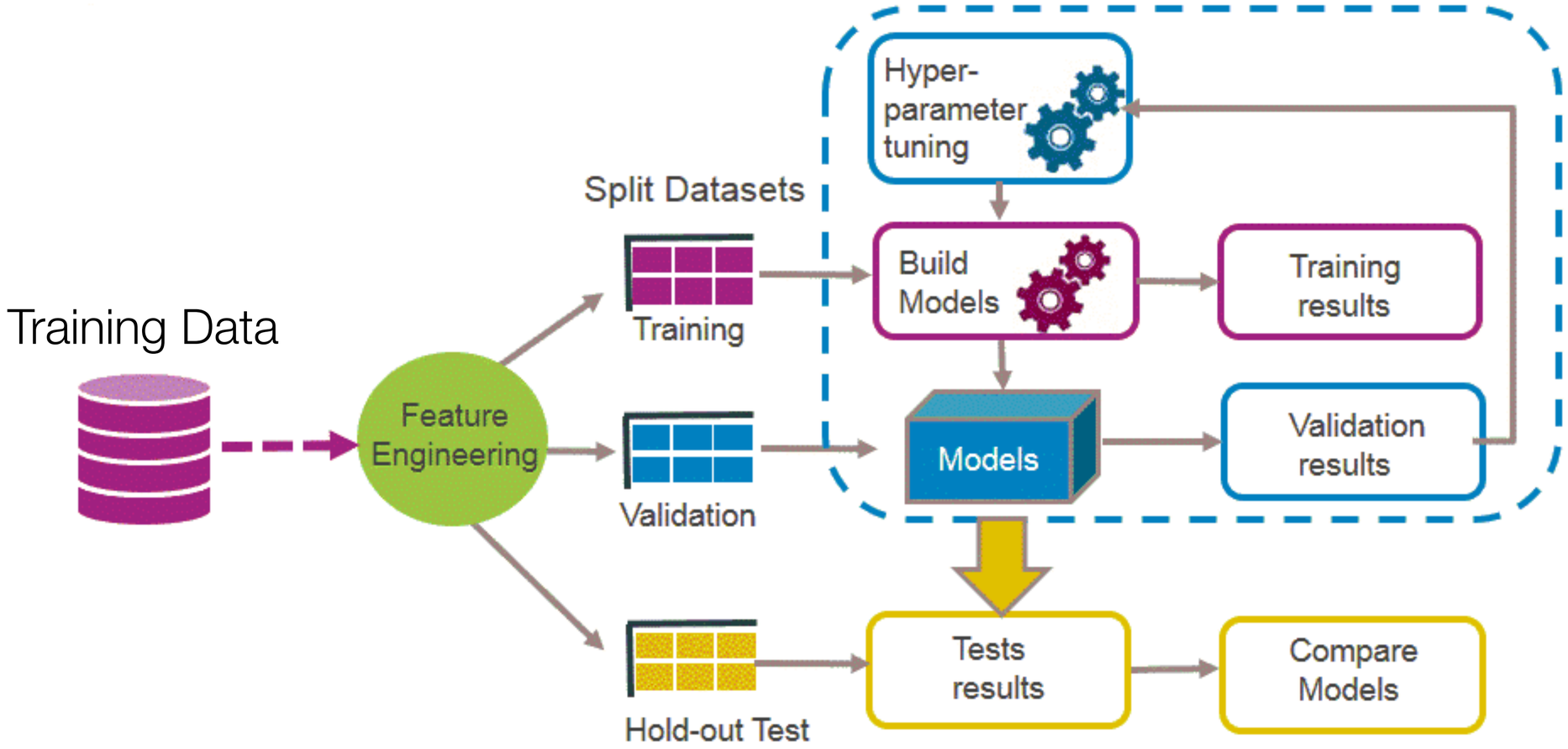
https://www.the-modeling-agency.com/crisp-dm.pdf

How do machines learn?

Lecture 2

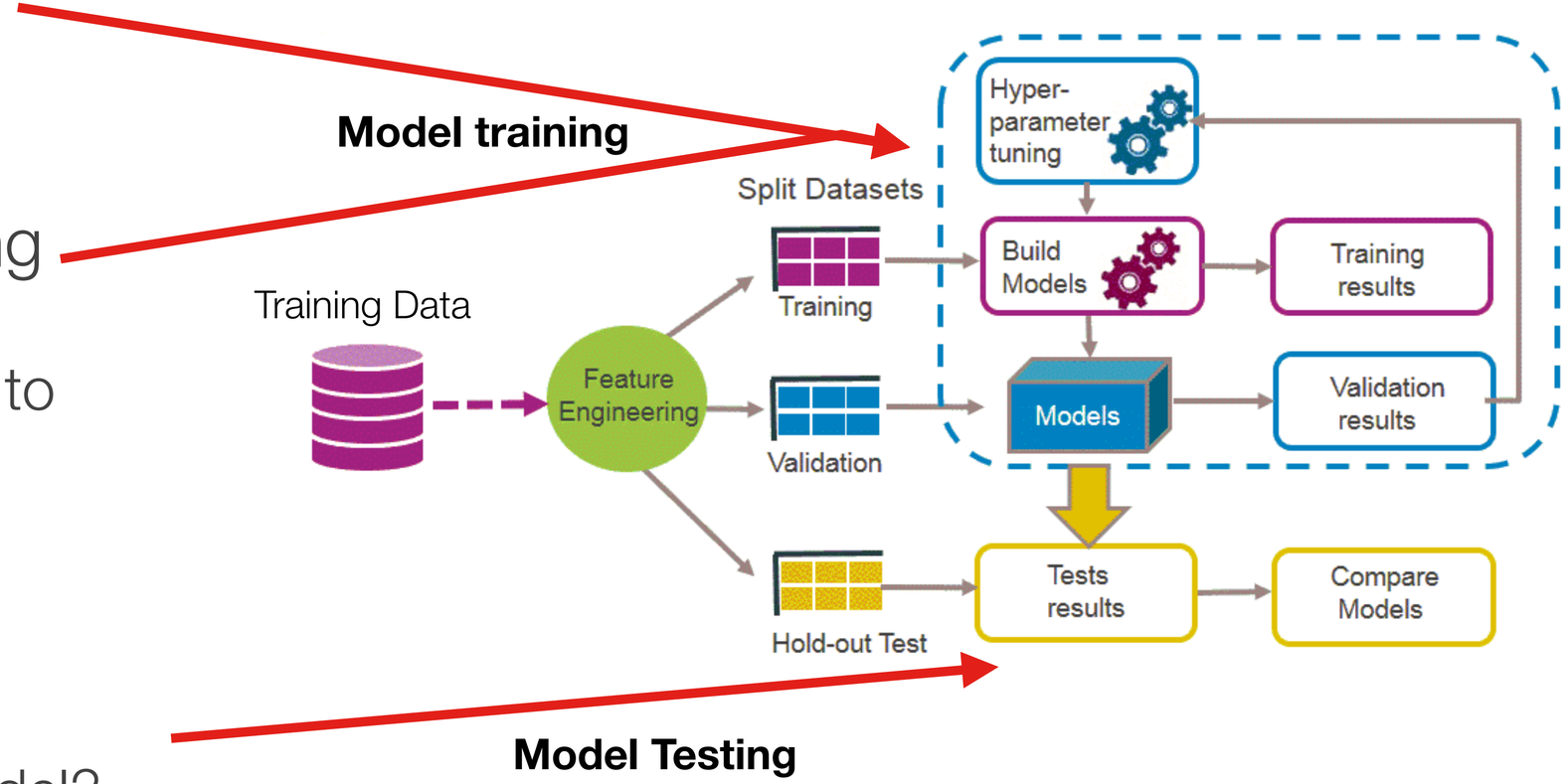


Machine Learning Training and Evaluation Process



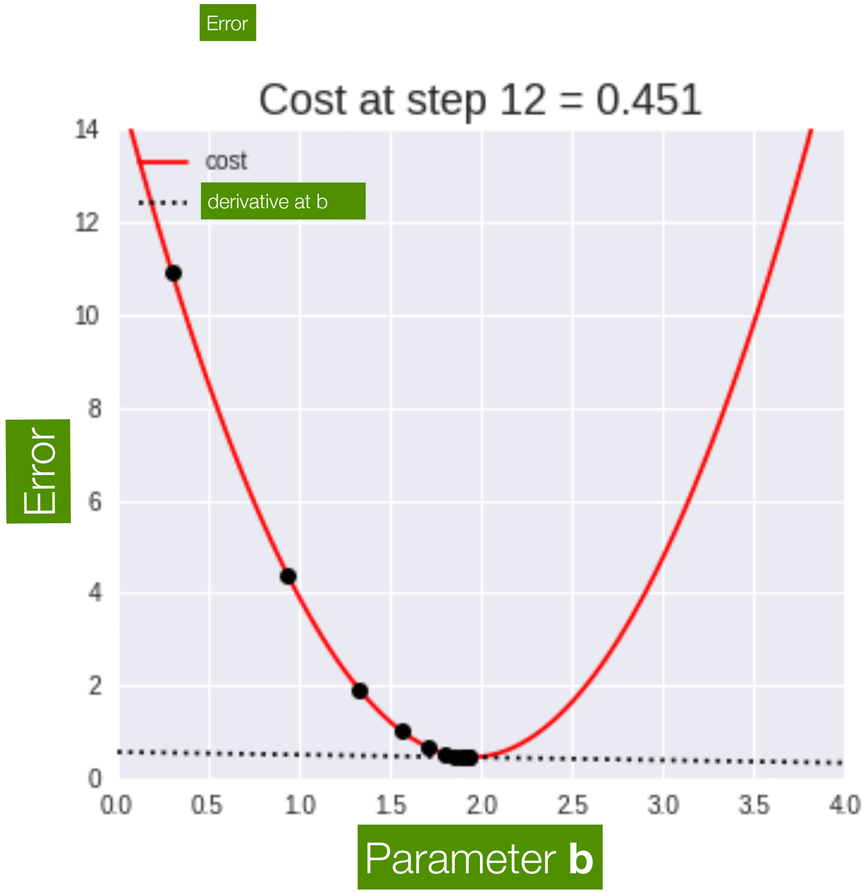
How to Evaluate?

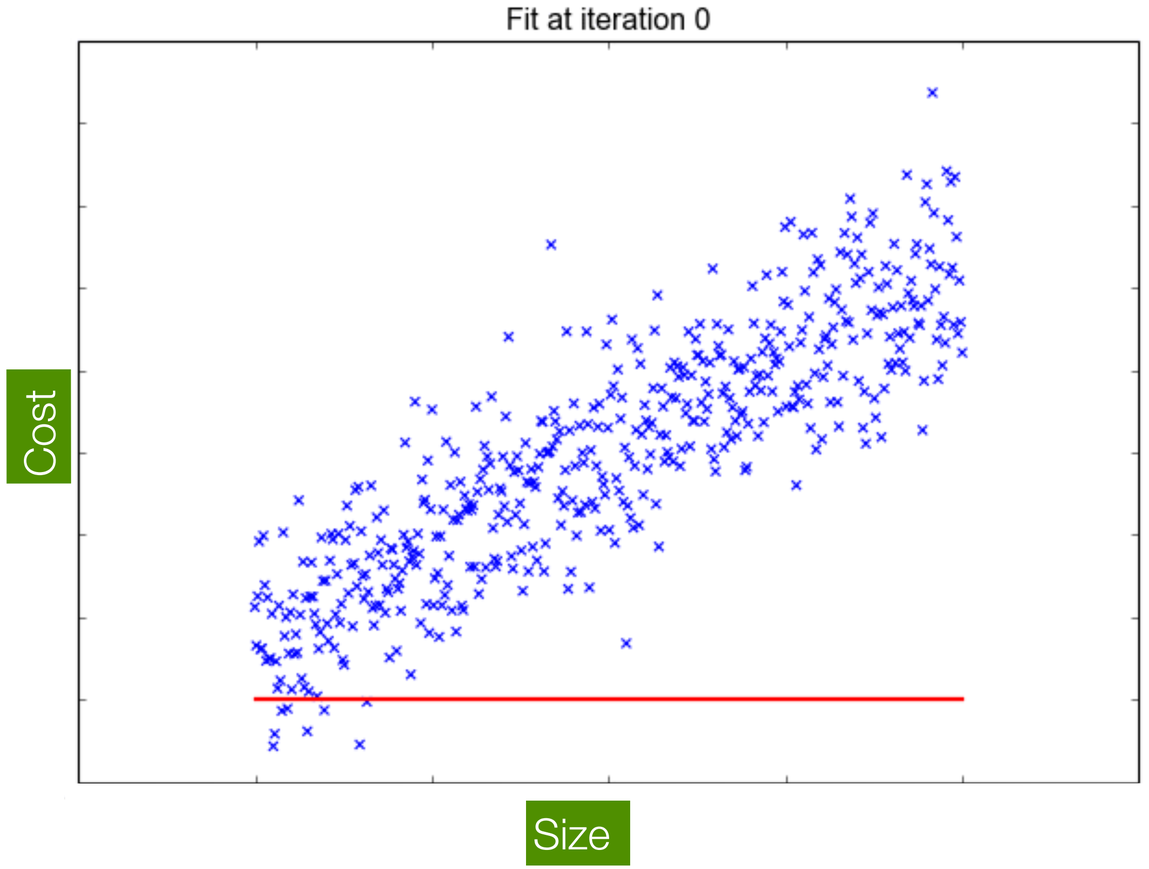
- Metric
  - How to measure errors?
  - Both training and testing
- Training of Machine Learning algorithm
  - How to “help” the ML model to generalise?
- Experiment
  - How to pick the best ML model?



Training the model

Gradient descent





Model Training: Metric

- Errors are almost inevitable!
  - How to measure errors?

- We're generally interested in the following:
  - How often is the prediction wrong?
  - How is the prediction wrong?
  - What is the cost of wrong predictions?
  - How does the cost vary by the type of prediction that was wrong?
  - How can we minimize costs? (or regret?)

- Select an evaluation procedure (a "metric")
  - **Ok, but which one?**

Regression

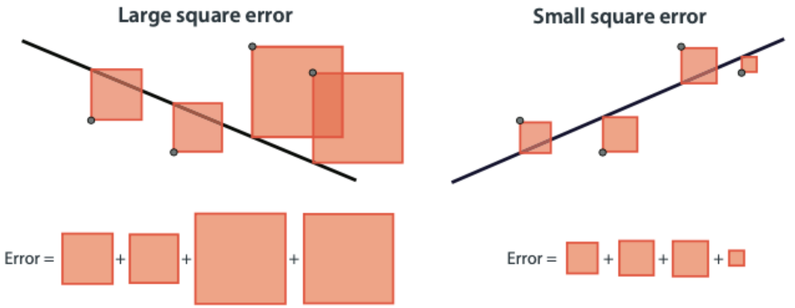
- **Mean (absolute | square) error**

- **Absolute**: average of the difference between the original values and the predicted value
  - No direction

$$MAE = \frac{1}{N}\sum_{J=1}^{N} |prediction_j - value_j|$$

- **Square**: average of the square of the difference between the original values and the predicted value
  - Square is *nicer* to deal with during the training process (derivative)
  - Larger errors are more pronounced

$$MSE = \frac{1}{2N}\sum_{J=1}^{N} (prediction_j - value_j)^2$$

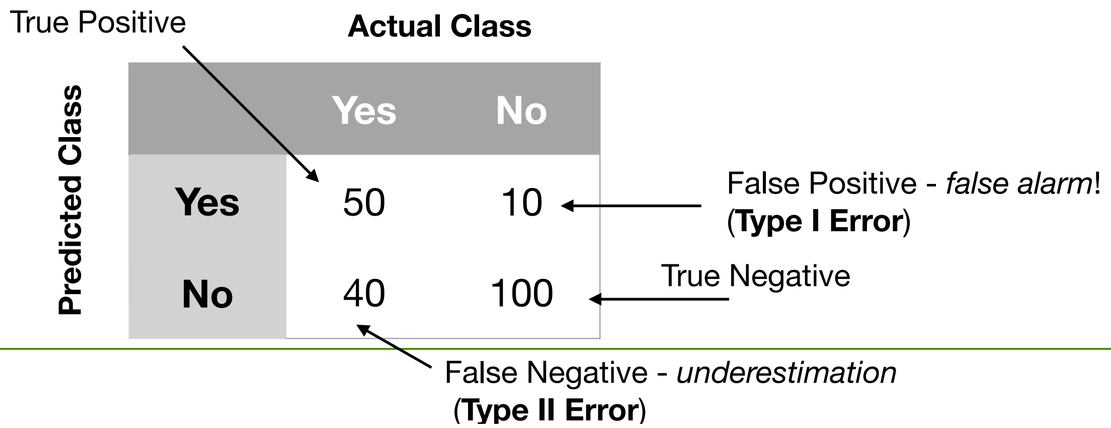


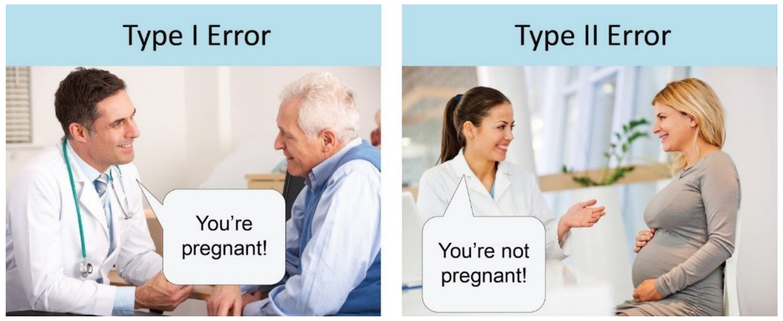
Classification

- **Accuracy**
  - The percentage of times that a model is correct
  - However, the model with the highest accuracy is not necessarily the best model
  - Some errors (e.g. False Negative) may be much more expensive than others
    - Usually due to imbalanced trained datasets

$$Accuracy = \frac{\#CorrectPredictions}{\#Predictions}$$

- **Confusions Matrix**
  - Describes the complete performance of the model





$$Accuracy = \frac{\#TruePositives + \#TrueNegatives}{\#AllPredictions}$$

All errors are not equal

- Depending on your task, different errors have different costs

- Pregnancy detection
  - Cost of “false negatives”?
  - Cost of “false positives”?

- Covid testing
  - Cost of “false negatives”?
  - Cost of “false positives”?

- In law enforcement?

- In detecting the “Alexa” command?
- In detecting a person on the road?

FALSE POSITIVES: SELF-DRIVING CARS AND THE AGONY OF KNOWING WHAT MATTERS

According to a preliminary report released by the National Transportation Safety Board last week, Uber’s system detected pedestrian Elaine Herzberg six seconds before striking and killing her. It identified her as an unknown object, then a vehicle, then finally a bicycle. (She was pushing a bike, so close enough.) About a second before the crash, the system determined it needed to slam on the brakes. But Uber hadn’t set up its system to act on that decision, the NTSB explained in the report. The engineers prevented their car from making that call on its own “to reduce the potential for erratic vehicle behavior.” (The company relied on the car’s human operator to avoid crashes, which is a whole separate problem.)

ARN MORE

Uber’s engineers decided not to let the car auto-brake because they were worried the system would overreact to things that were unimportant or not there at all. They were, in other words, very worried about false positives.

https://www.wired.com/story/self-driving-cars-uber-crash-false-positive-negative/

Classification

- **Precision**
  - Among the examples we classified as positive, how many did we correctly classify?
- **Recall**
  - Among the positive examples, how many did we correctly classify?

$$Precision = \frac{TruePositive}{TruePositive + FalsePositive}$$

$$Recall = \frac{TruePositive}{TruePositive + FalseNegative}$$

- **F1-Score**
  - The harmonic mean between **precision** (how many instances correctly classified), and **recall** (how many relevant instances are correctly classified)

$$F_1 = 2 * \frac{1}{\frac{1}{Precision} + \frac{1}{Recall}}$$

  - What is the implicit assumption about the costs of errors?

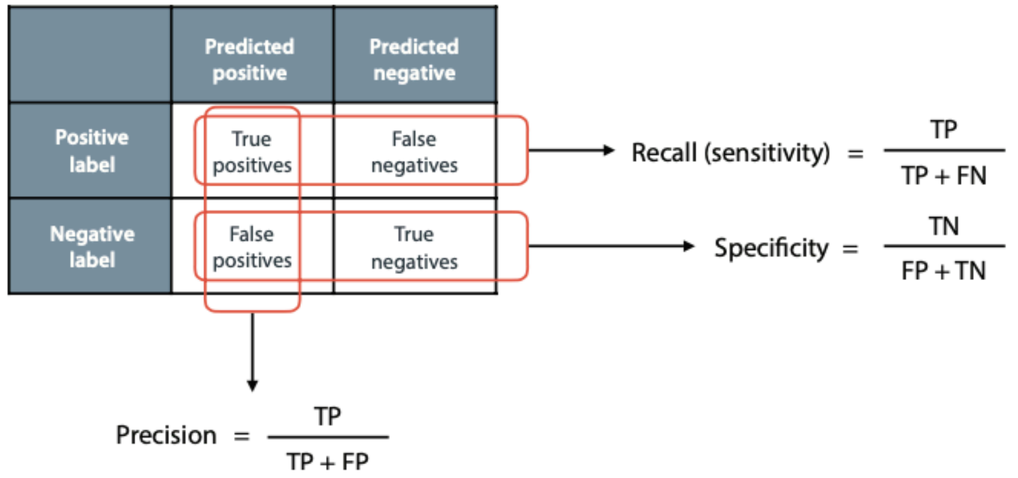
Classification

- **Sensitivity** (True positive rate)
  - the capacity of the model to identify the positively labelled points
  - Same as recall

$$Sensitivity = \frac{TruePositive}{FalseNegative + TruePositive}$$

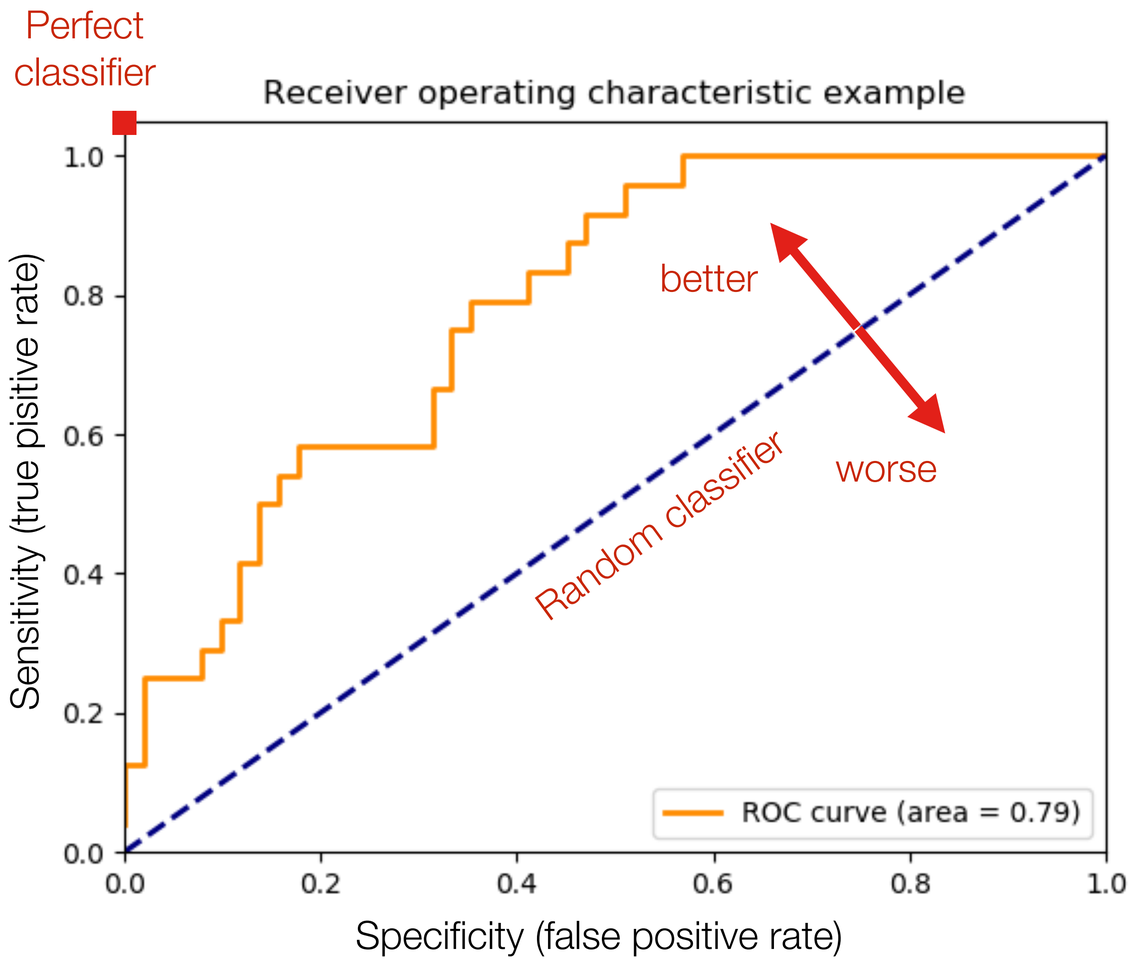
- **Specificity** (False positive rate)
  - the capacity of the model to identify the negatively labeled points
  - Not the same as precision

$$Specificity = \frac{TrueNegative}{FalsePositive + TrueNegative}$$



The receiver operating characteristic (ROC) curve

- A useful technique to evaluate a model based on its performance on false positives and negatives at the same time
  - based on *sensitivity* and *specificity*
- It also gives us a way to "explore" model performance visually
  - Trade-off specificity and sensitivity by moving the threshold



Some Examples

- Medical model:
  - **Recall** and **sensitivity**: among the sick people (positives), how many were correctly diagnosed as sick?
  - **Precision**: among the people diagnosed as sick, how many were actually sick?
  - **Specificity**: among the healthy people (negatives), how many were correctly diagnosed as healthy?
- Email model:
  - **Recall** and **sensitivity**: among the spam emails (positives), how many were correctly deleted?
  - **Precision**: among the deleted emails, how many were actually spam?
  - **Specificity**: among the ham emails (negatives), how many were correctly sent to the inbox?

Choosing Metrics

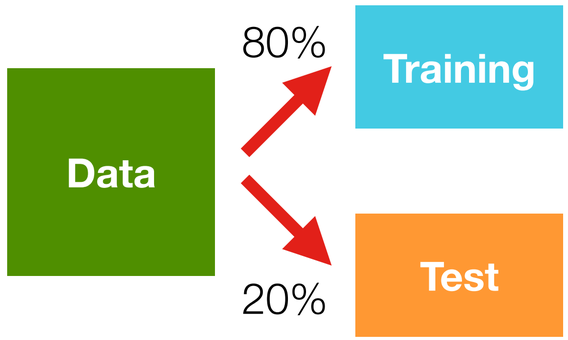
- If a high precision is a hard constraint, do the best recall
  - search engine results, grammar correction: Intolerant to FP
  - Metric: Recall at Precision = XX %

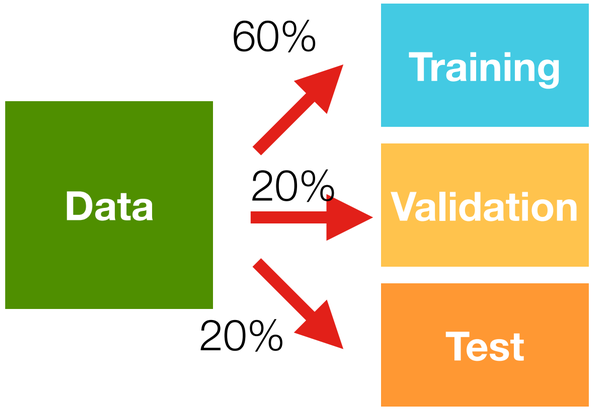
- If a high recall is a hard constraint, do best precision
  - medical diagnosis: Intolerant to FN
  - Metric: Precision at Recall = 100 %

- Capacity constrained (by K)
  - Metric: Precision in top-K

Model Training: dataset splitting

- Split your data
  - Training set —> to **train** the model
  - (Optional) Validation set —> to decide which model to use
  - Test set —> to evaluate the model

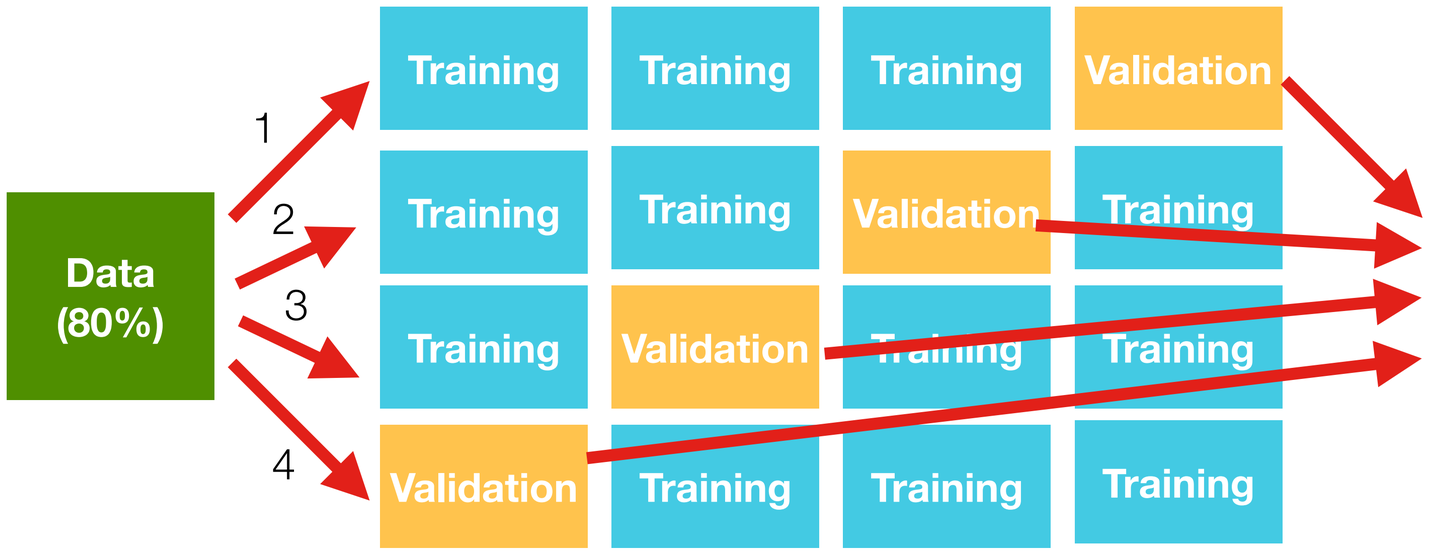




NEVER use the test set for training —> That is CHEATING!

Model Training: Cross-validation

- A way to use all the data for training and testing, by recycling it several times
  - Splitt the data in *n* portions
  - Train the model *n* times using *n-1* portions for training
- Useful when dataset is small



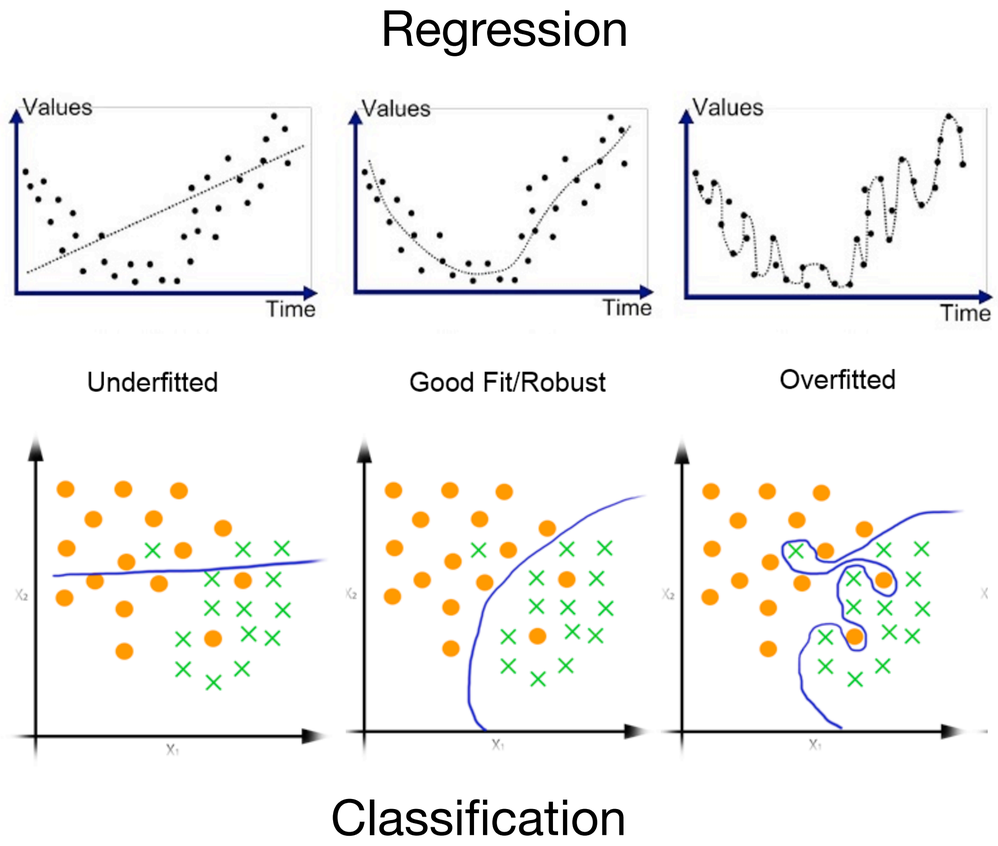
$$Score = \frac{Score_1 + Score_2 + Score_3 + Score_4}{4}$$

Example: four-fold cross-validation

No free-lunch

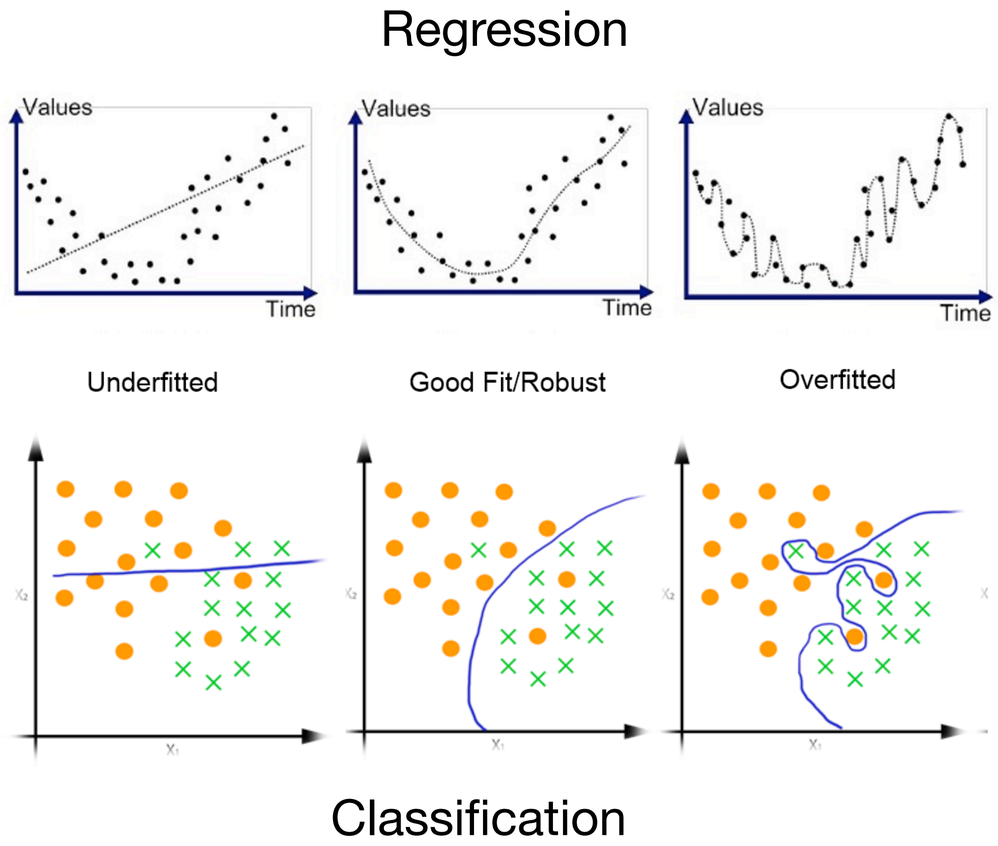
- There is no one best machine learning algorithm for all problems and datasets

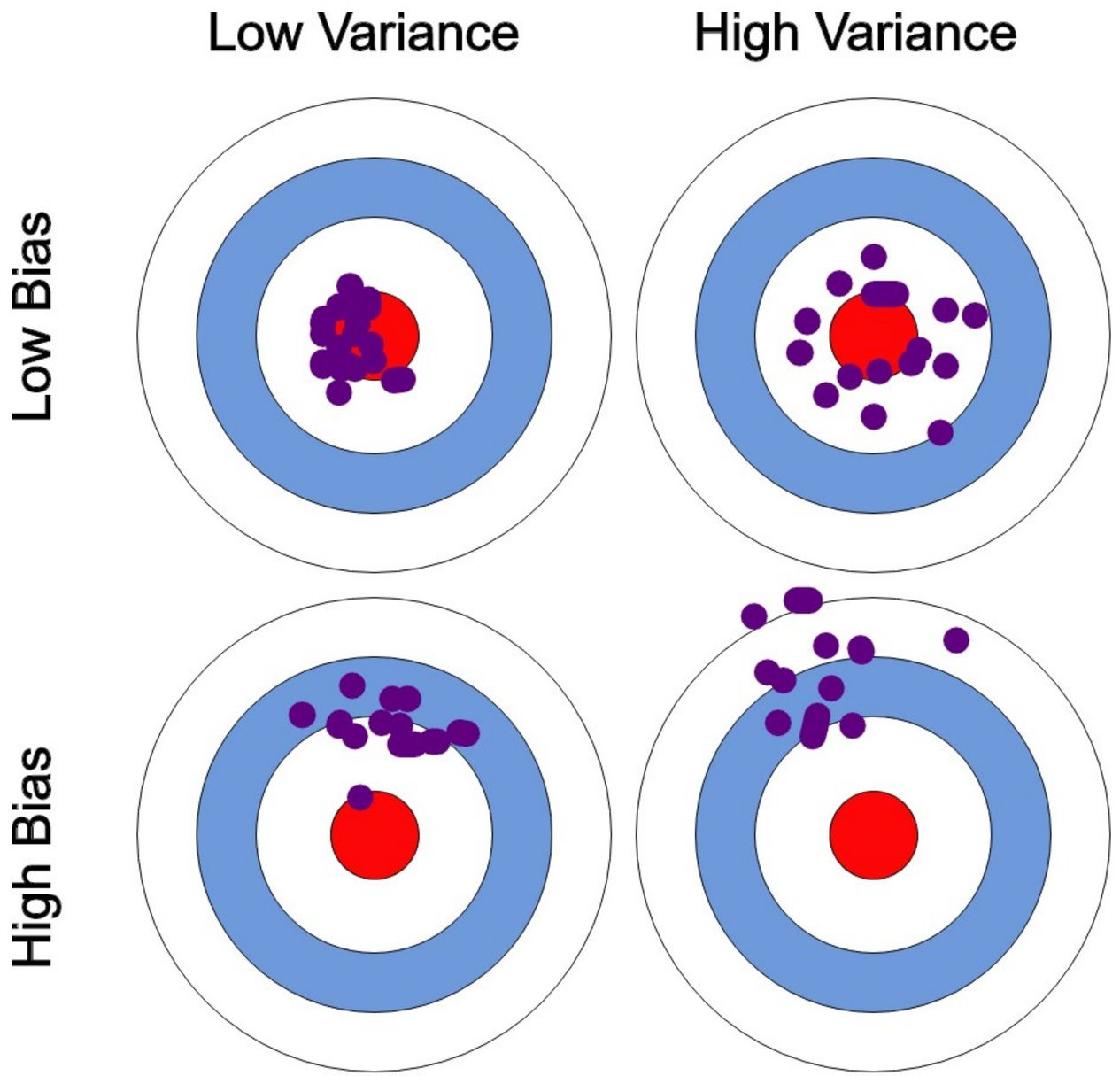
- **Generalisation**
  - How well does a learned model generalize from the data it was trained on to a new evaluation set?



Generalisation

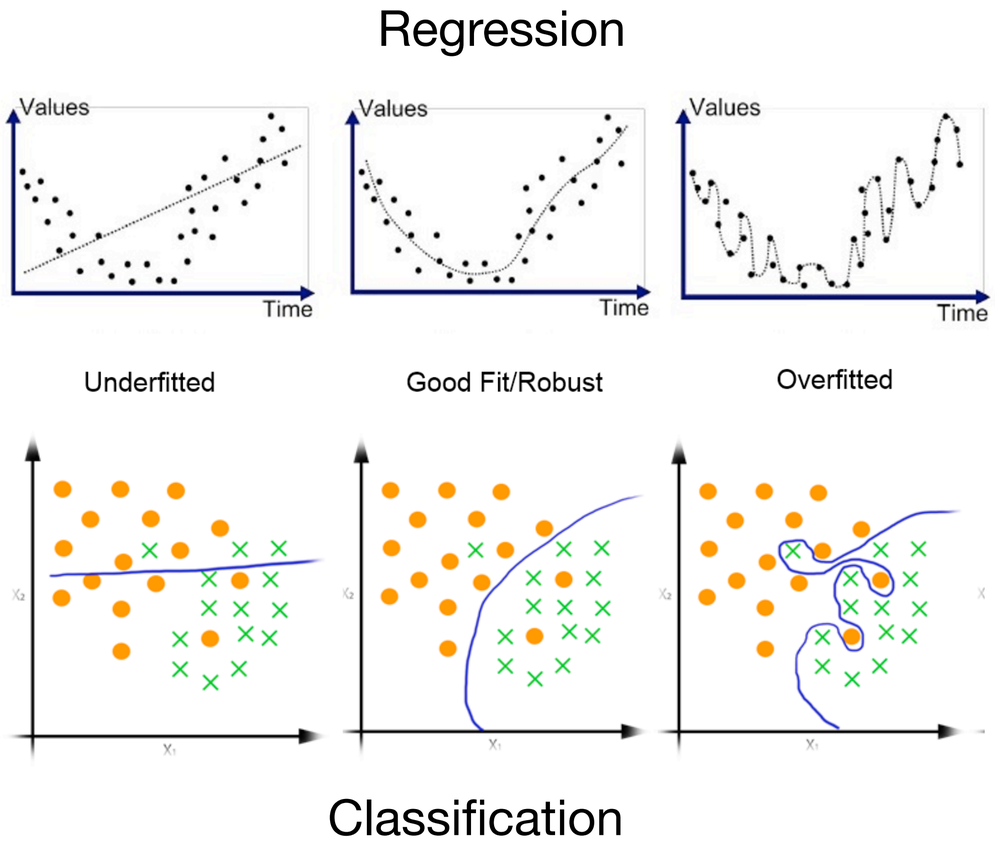
- **Challenge**: achieving good generalization and a small error rate
- Components of expected loss
  - **Noise** in our observations: **unavoidable**
  - **Bias**: how much the average model overall training sets differs from the true model
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance**: how much models estimated from different training sets differ from each other
    - Too much sensitivity to the samples




Low Variance
High Variance
Low Bias
High Bias

Overfitting vs. Underfitting

- Protect against **overfitting**
  - learning a model that too closely matches the idiosyncrasies of the training data
  - model is too “complex” and fits irrelevant characteristics (noise) in the data
    - Low bias and high variance
    - Low training error and high test error
- Protect against **underfitting**
  - learning a model that does not adequately capture the patterns in the training data
  - The model is too “simple” to represent all the relevant class characteristics
    - High bias and low variance
    - High training error and high test error



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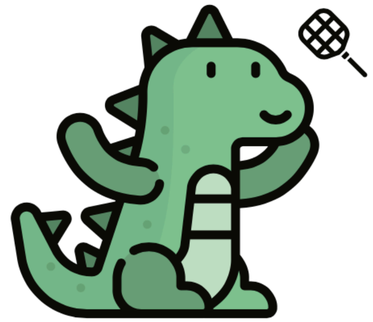
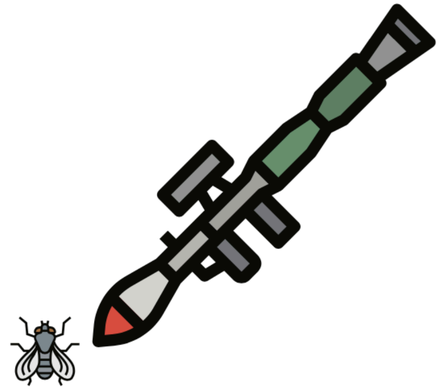
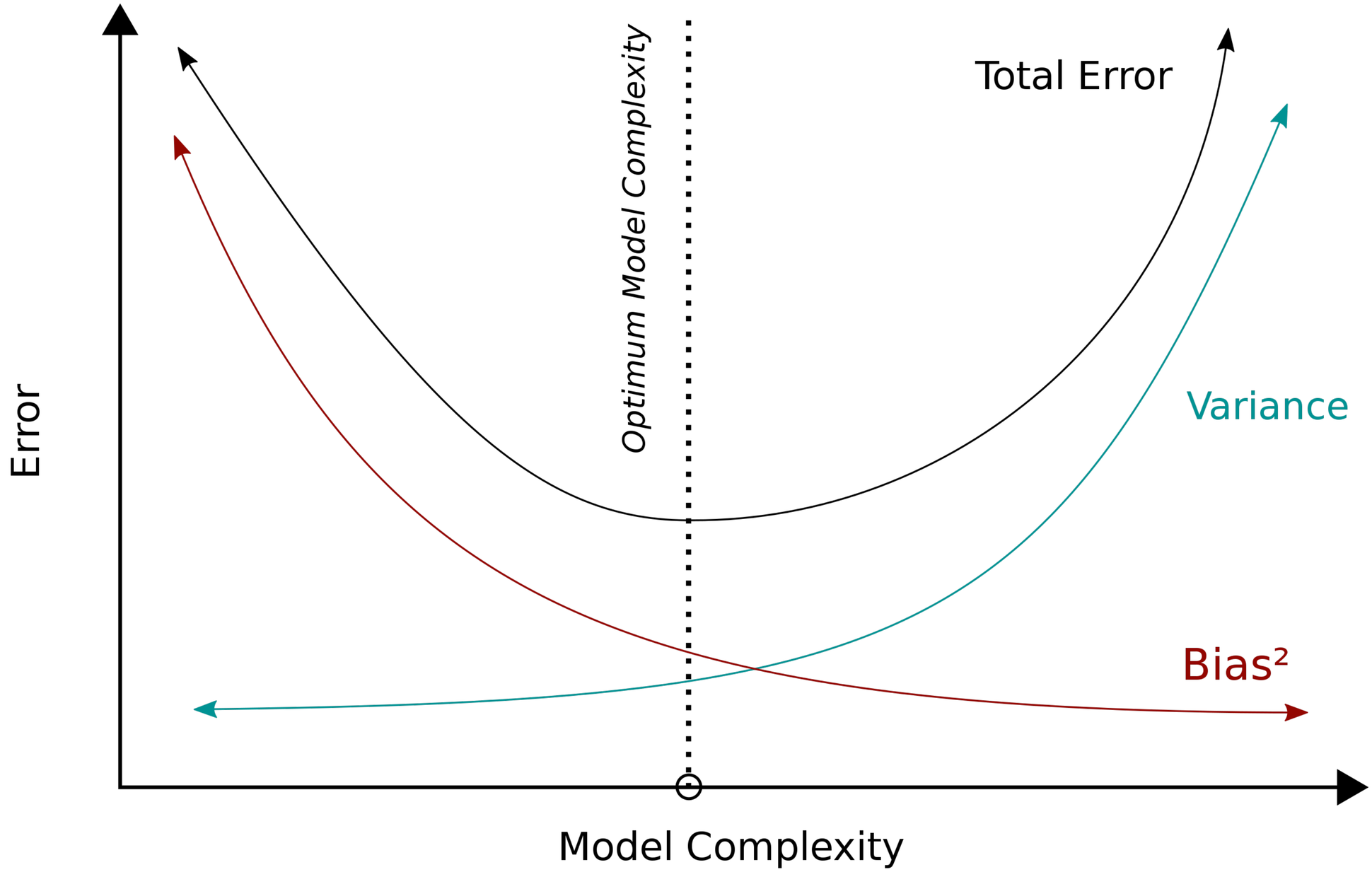


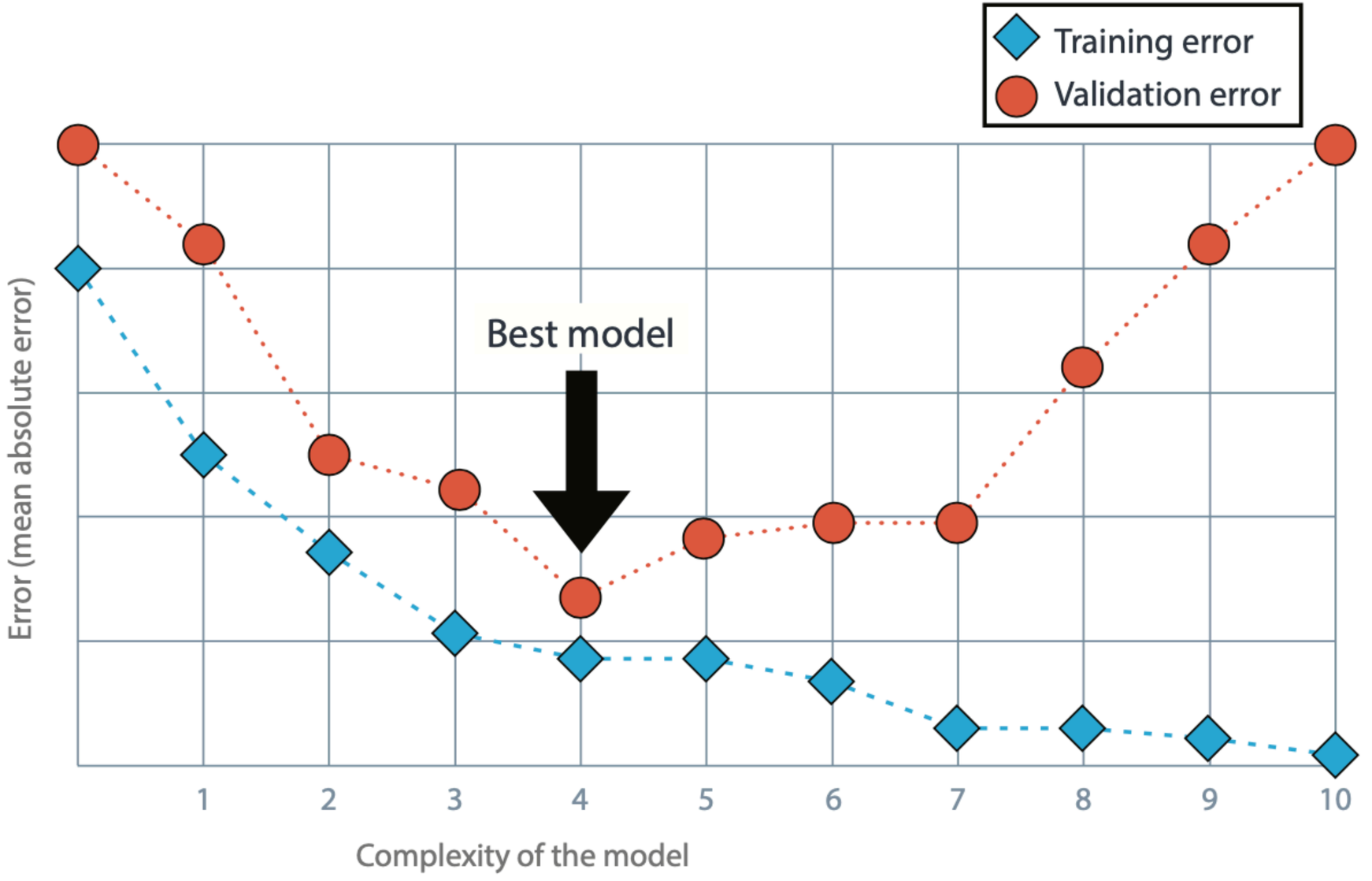
Underfitting



Overfitting

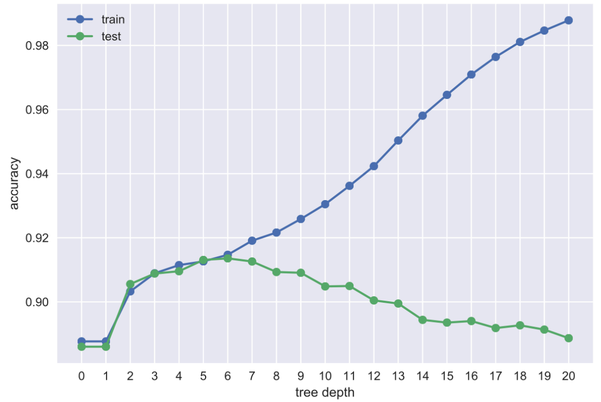


https://en.wikipedia.org/wiki/Bias–variance_tradeoff#/media/File:Bias_and_variance_contributing_to_total_error.svg


Training error
Validation error
Best model
Error (mean absolute error)
1
2
3
4
5
6
7
8
9
10
Complexity of the model

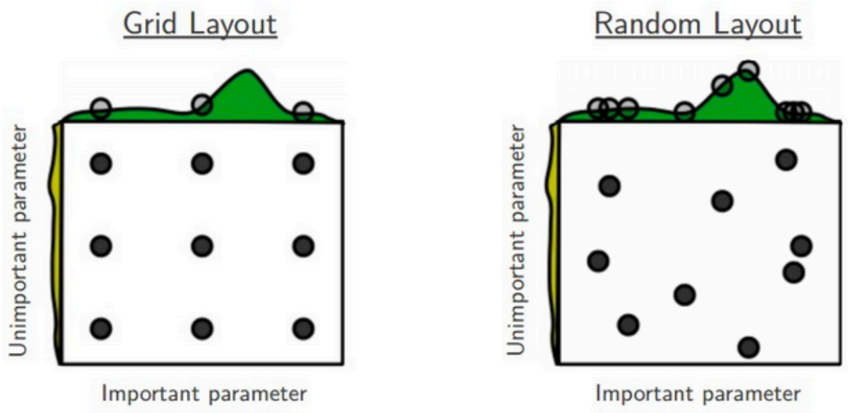
Tuning Hyperparameters

- Inputs to the learning algorithms that control their behaviour
  - Examples:
    - maximum tree depth in decision trees
    - number of neighbours *k* in *k-nearest neighbour*
    - Neural networks: architecture, learning rate



- For a model to work well, they often need to be tuned carefully
  - Huge search space! may be inefficient to search exhaustively

- Possible approaches
  - **Grid search**: brute-force exhaustive search among a finite set of hyperparameter settings
    - All combinations are tried, then the best setting selected
  - **Random search**: for each hyperparameter, define a distribution (e.g. normal, uniform)
    - In the search loop, we sample randomly from these distributions

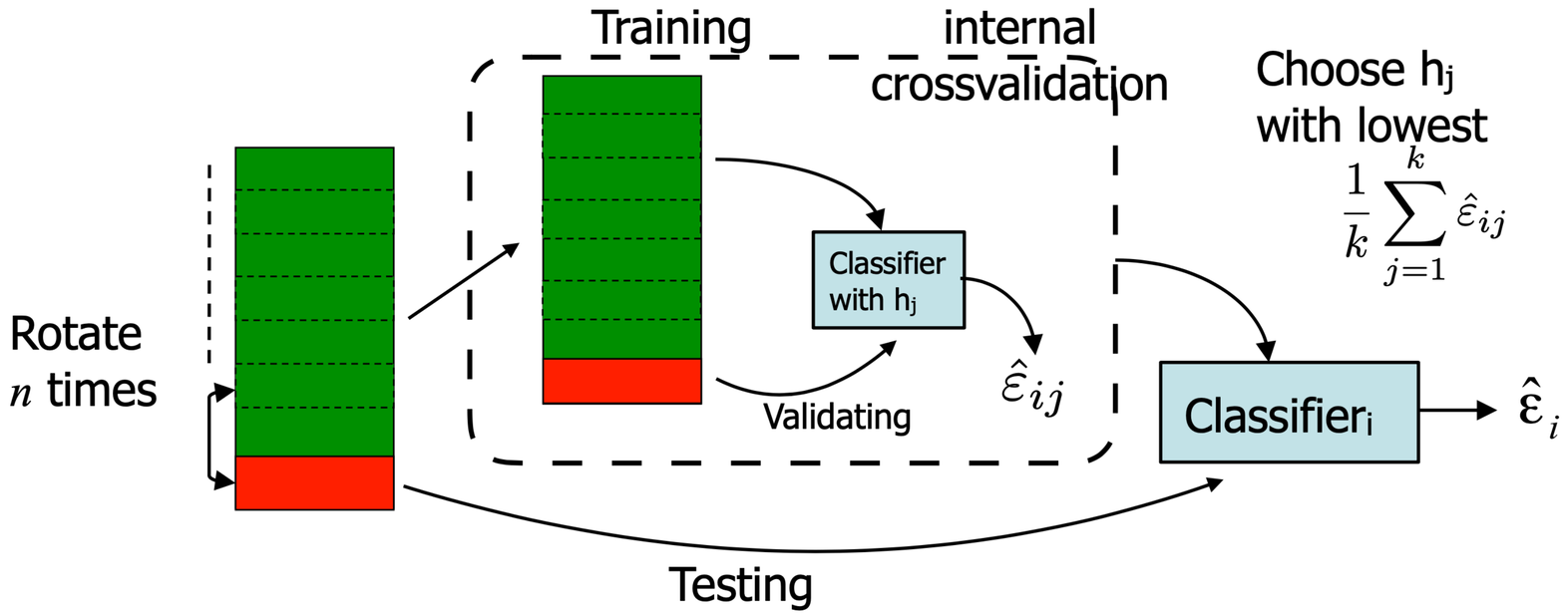


https://www.jmlr.org/papers/volume13/bergstra12a/bergstra12a

DON'T optimise these numbers by looking at the test set! That is CHEATING!

Double Cross-Validation

- To optimise over the hyperparameter do cross-validation inside another cross-validation
- The minimum error is often not the most interesting. Try to understand the advantages/disadvantages
  - What errors are made? (inspect objects, inspect labels)
  - What classes are problematic? (confusion matrix)
  - Does adding training data help? (learning curve)
  - How robust is the model?



Model Evaluation: Experiments

- Compare to one or more baselines
  - Existing solution
  - Trivial (new) solution
  - Rule-based solution
  - Multiple ML models

More next week

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Credits

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- https://scikit-learn.org/stable/modules/tree.html
- CIS 419/519 Applied Machine Learning. Eric Eaton, Dinesh Jayaraman. https://www.seas.upenn.edu/~cis519/spring2020/