Evaluation II

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Outline

- Evaluation
- Overfitting
- Model Bias and Variance
- Evaluation Bias and Variance

Evaluation of Supervised ML

- Start with a dataset of instances comprised of attributes and labels
- Build a classifier using a learner and the dataset
- Assess the effectiveness of the classifier
  - Comparing the predictions with the actual labels on unseen instances
  - Metrics: accuracy, precision, recall, F1-score

Inductive Learning Hypothesis

- Any hypothesis found to approximate the target function well over *a sufficiently large training data set* will also approximate the target function well over *held-out test examples*.

  - What does it mean by “large training data set”?
  - Why do we need to test our hypothesis on “held-out test examples”?
  - What impact does the size of the test set have?

Tensions in Classification

Our evaluations must take these ideas into consideration

- **Consistency**: is the classifier able to flawlessly predict the class of all training instances?
- **Overfitting**: has the classifier tuned itself to the training data rather than learning its generalisable properties?
- **Generalisation**: how well does the classifier generalise from the specifics of the training examples to predict the target function?

Overfitting

Learning Curves

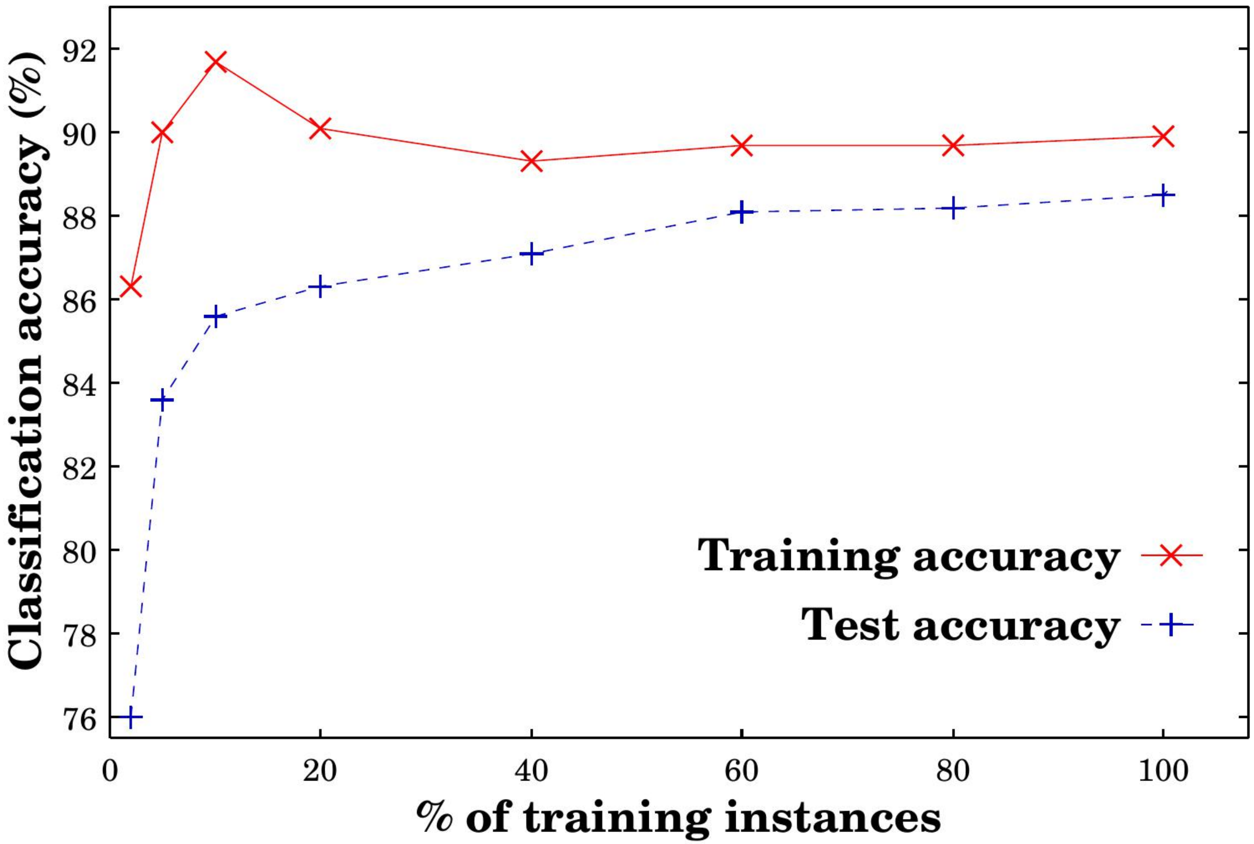
- Learning curve is a plot of learning performance over experience or time
- For machine learning models, we can plot:
  - **y-axis**: performance measured by accuracy, error or other metrics
  - **x-axis**: conditions, e.g. sizes of training sets, model complexity, iterations…
  - **Training** learning curve: calculated from the *training* set that shows how well the model is *learning*.
  - **Test** learning curve: calculated from a *holdout* set that shows how well the model is *generalising*.

Learning Curves

Example 1: for different sizes of training set

- Choose various split sizes, and calculate effectiveness
  - For example: 90-10, 80-20, 70-30, 60-40, 50-50, 40-60, 30-70, 20-80, 10-90 (9 points)
  - Might need to average multiple runs per split size
- Plot % of training data vs training/test accuracy (or other metric)
- Benefit: allows us to visualise the data trade-off
  - More training instances?
  - More evaluation instances?

Learning Curves



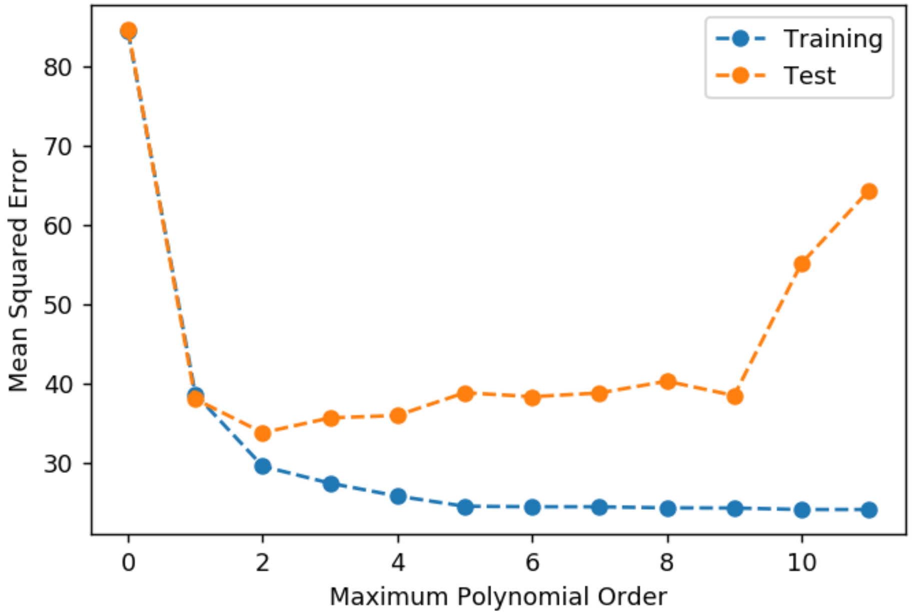
Learning Curves

Example 2: compare models

- Using the polynomial of x to increase the flexibility of linear regression

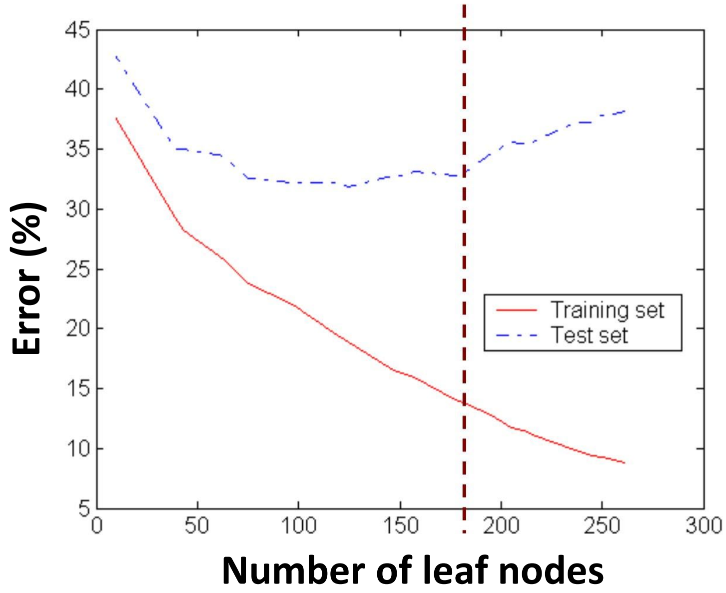
$$y = \boldsymbol{w} \cdot \phi(x)$$

$$\phi(x) = [1, x, x^2, \dots, x^D]$$



Overfitting

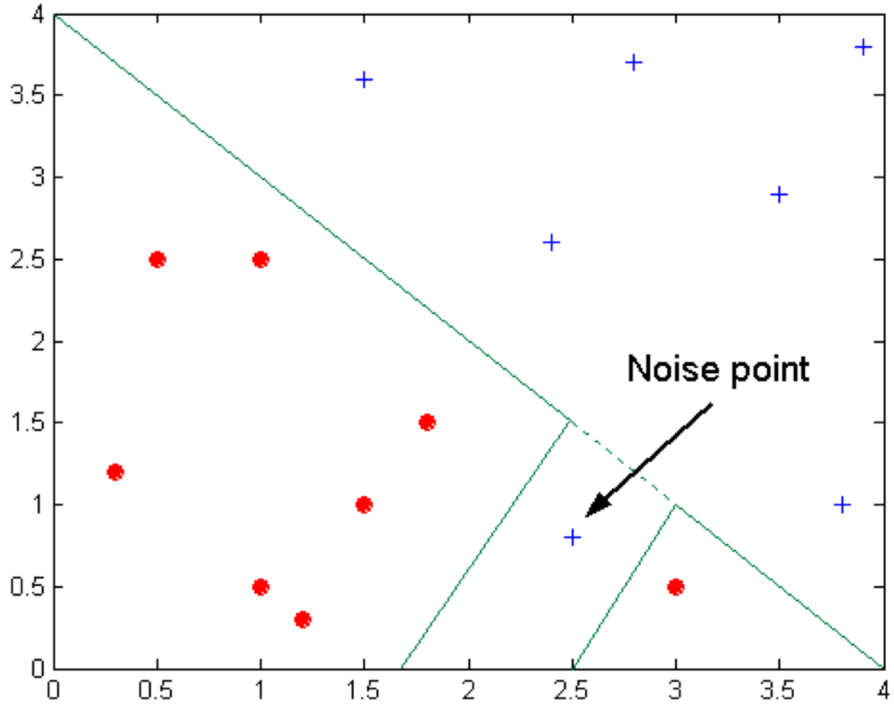
- An overly complex model is selected that captures specific patterns in the training data but fails to learn the true nature of relationships between attributes and class labels
- Possible evidence of overfitting



large gap between training and test performance

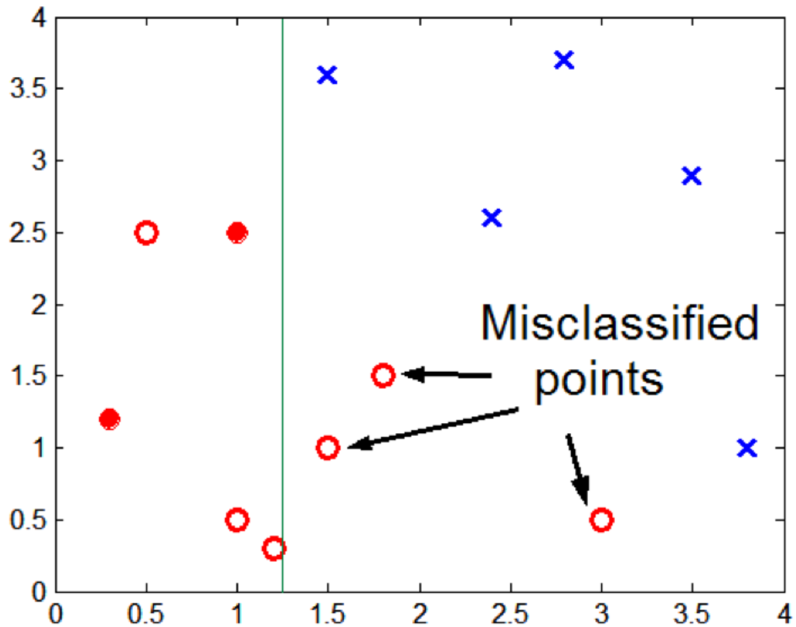
Reasons of Overfitting

- Decision boundary distorted by noise
- A simpler decision boundary would generalise better for this data



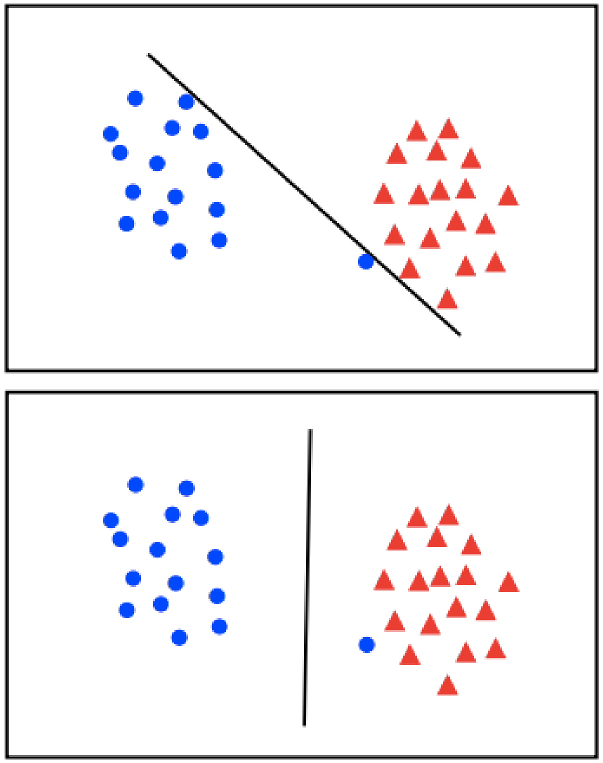
Reasons of Overfitting

- Limited training set: not fully represent the patterns in the population
  - could be due to small number of examples
  - could be due to non-randomness in training samples (sampling bias)



Solution: Regularisation

- In soft-margin SVM, the slack variables provide regularisation



$$\min_{\boldsymbol{w}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N}\xi_i$$

$$\text{subject to } y_i\left(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_i + b\right) + \xi_i - 1 \geq 0,$$

$$\xi_i \geq 0, \forall\, i \in \{1,2,\ldots,N\}$$

Solution: Regularisation

- In linear regression, the norm of the parameters can be used as regulariser
- Mathematically, a norm is a total length of a vector. The L_p norm of $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_k, \ldots, \beta_D]$ is defined as:

$$\|\boldsymbol{\beta}\|_p = \sqrt[p]{\sum\nolimits_k |\beta_k|^p}$$

- Optimisation objective function:

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}}[Error(\boldsymbol{\beta}; \{\boldsymbol{X}, Y\}) + \lambda\psi(\boldsymbol{\beta})]$$

  - $\lambda (> 0)$ is a hyperparameter, tuned empirically through trial-and-error
  - $\psi(\boldsymbol{\beta})$ is regulariser

Solution: Regularisation

- Linear regression with L2-norm regularisation (ridge regression)

$$\psi(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_2^2 = \sum_k |\beta_k|^2$$

  - penalises parameter values by adding the sum of their *squared* values to the error term
  - encourages solutions where most parameter values are *small*

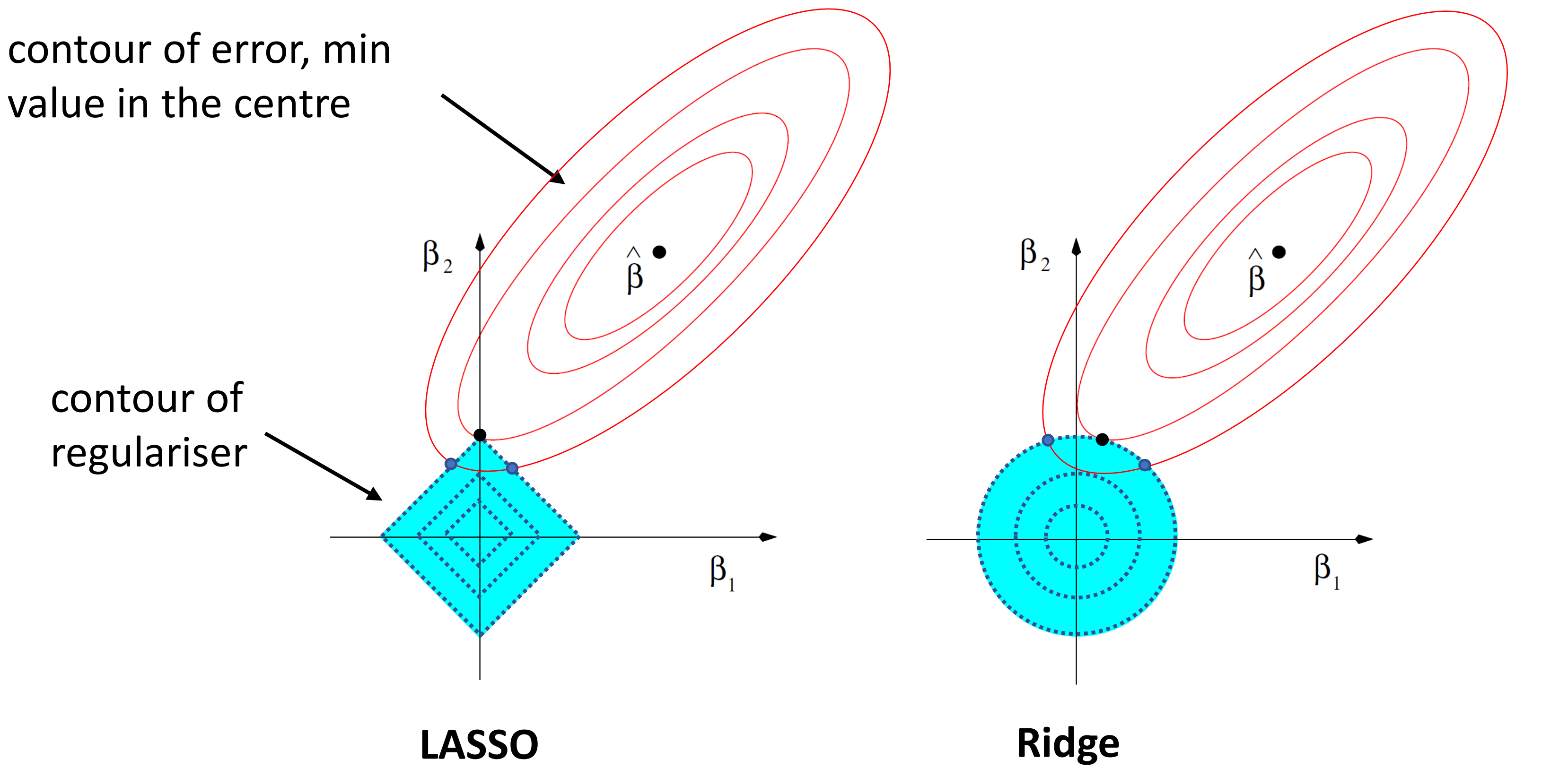
- Linear regression with L1-norm regularisation (LASSO)

$$\psi(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_1 = \sum_k |\beta_k|$$

  - penalises parameter values by adding the sum of their *absolute* values to the error term
  - encourages solutions where few parameters are non-zero

Solution: Regularisation

- Comparison of ridge regression and LASSO



Model Bias and Variance

Bias and Variance

- Statistical definition: the bias and variance of estimation $\hat{\theta}$ for true θ are

$$Bias(\hat{\theta}, \theta) = E[\hat{\theta}(x) - \theta(x)]$$

$$Var(\hat{\theta}, \theta) = E[(\hat{\theta}(x) - E[\hat{\theta}(x)])^2]$$

Bias and Variance

In machine learning

- Bias is used to refer to a number of things:
  - Model bias: the tendency of our model to make systematically wrong predictions
  - Evaluation bias: the tendency of our evaluation strategy to over- or under-estimate the effectiveness of our model
  - Sampling bias: if our training or evaluation dataset isn't representative of the population, which breaks the Inductive Learning Hypothesis
- Variance refers to model variance and evaluation variance

Model Bias and Variance

- **Model bias** in **regression** context:
  - For every evaluation instance, the signed error can be calculated
  - Assuming every instance is independent, bias is the average of these signed errors

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)$$

- A model is **biased** if
  - the predictions are systematically *higher* than the true value, or
  - the predictions are systematically *lower* than the true value
- A model is **unbiased** if
  - the predictions are systematically correct, or
  - some of the predictions are too high, and some of the predictions are too low

Model Bias and Variance

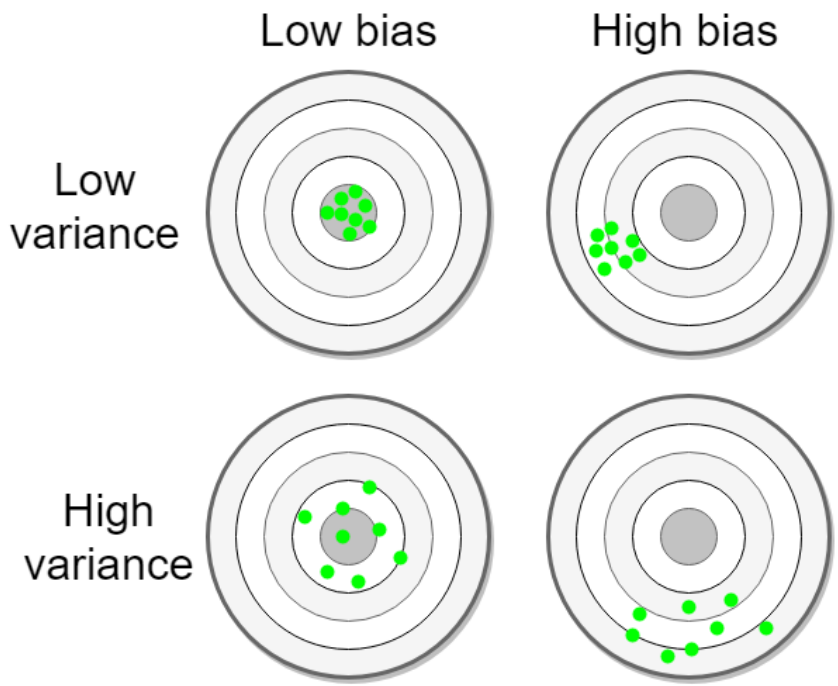
- **Model bias** in **classification** context:
  - Label predictions can't be "too high" or "too low"
  - "biased towards the majority class" means our model predicts too many instances as the majority class

  - Typically compare the class distribution:
    - An **unbiased** classifier produces labels with the same distribution as the actual distribution
    - A **biased** classifier produces labels with a different distribution from the actual distribution

Model Bias and Variance

- **Model variance** relates to the tendency of different training sets to produce different models or predictions with the same type of learner
  - A model has **high variance** if a different randomly sampled training set leads to very different predictions on the evaluation set
  - A model has **low variance** if a different randomly sampled training set leads to similar predictions, independent of whether the predictions are correct

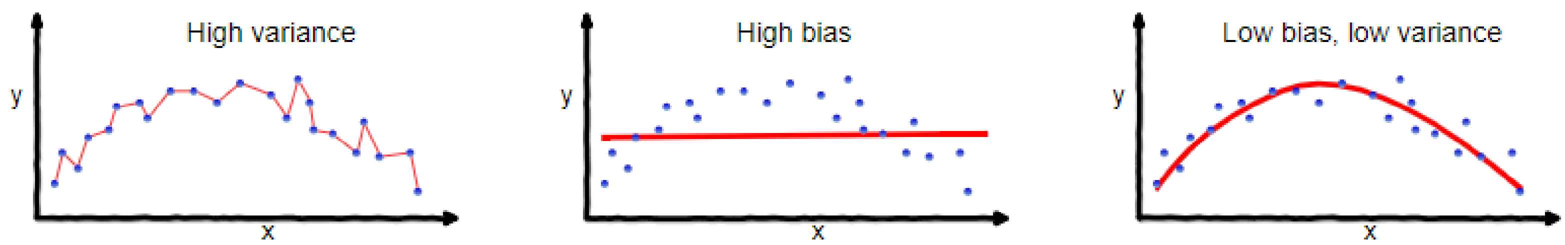
Model Bias and Variance



source: www.machinelearningtutorial.net/2017/01/26/the-bias-variance-tradeoff/

Model Bias and Variance

- High bias or high variance are bad
  - For example, 0-R has zero variance but high bias.
  - It is important to keep balance.
- Lower bias and lower variance --> better generalisation



overfitting   underfitting   Good balance

source: https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229/

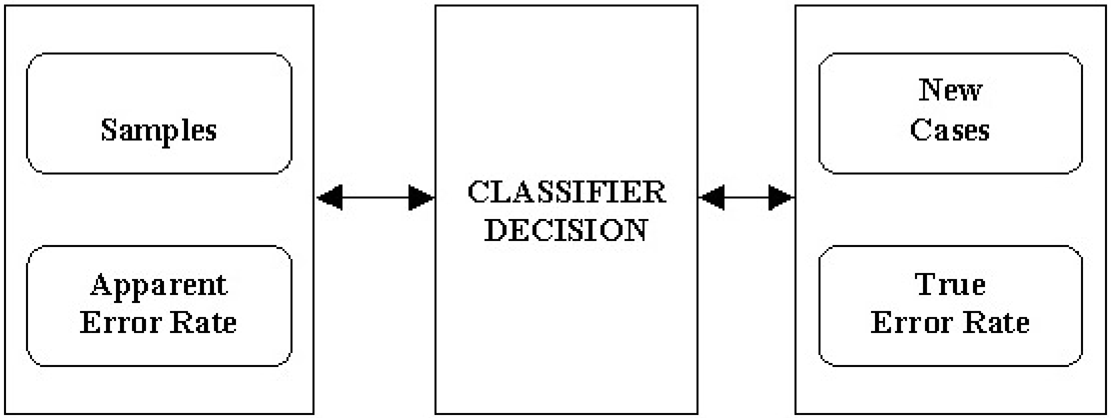
Evaluation Bias and Variance

Evaluation

- The evaluation metric is also an estimator
- Desire to know the *true error rate* of a classifier, but only have an estimate of the error rate, subject to some particular set of evaluation instances
- The quality of the estimation is independent of the trained model

Evaluation

- For example, training error is one starting point in estimating the performance of a classifier on new cases
- With *unlimited* samples, apparent error rate will become the true error rate



source: http://dms1.irb.hr/tutorial/tut_mod_eval_3.php

Evaluation Bias and Variance

- Evaluation bias

$$Bias(\hat{\theta}, \theta) = E[\hat{\theta}(x) - \theta(x)]$$

  - Our estimate of the effectiveness of a model is systematically too high/low

- Evaluation variance
  - Our estimate of the effectiveness of a model changes a lot, as we alter the instances in the test set
  - This can be hard to distinguish from model variance

Evaluation

How do we control bias and variance in evaluation?

- Holdout partition size
  - More training data: less model variance, more evaluation variance
  - Less training but more test data: more model variance, less evaluation variance
- Repeated random subsampling and K-fold Cross-Validation
  - Less variance than Holdout
- Stratification: less model and evaluation bias
- Leave-one-out Cross-Validation
  - No sampling bias, lowest bias/variance in general

Summary

- What is generalisation and overfitting?
- What is a learning curve, and why is it useful?
- How are bias and variance different?
- How is model bias different to evaluation bias?
- How do we try to control for bias and variance in evaluation?

References

Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar. Introduction to Data Mining. Pearson, 2018.