Final Exam

Time: Friday, 9 May, 9:45 pm – 12:00 pm (exam duration: 2 hours)

Where: On-campus (Using Inspera in-person)

- https://www.student.unsw.edu.au/exams/inspera
- BYOD (Bring your own Device)
  - Make sure it is fully charged before the exam

Questions: 32 MCQ (Theory and calculation, No coding)

- You can flag
- You can see the maximum mark available
- You can navigate
- Auto submission for questions is enabled
- Maximum mark: 50 (52 marks available: 50 marks + 2 extra marks)
- You MUST click the submit button at the end to exit the SBE environment

Materials allowed:

- Calculator (UNSW approved): https://www.student.unsw.edu.au/exam/calculators
- One A4 (2-sided cheat sheet)

Sample Test: Available on Moodle

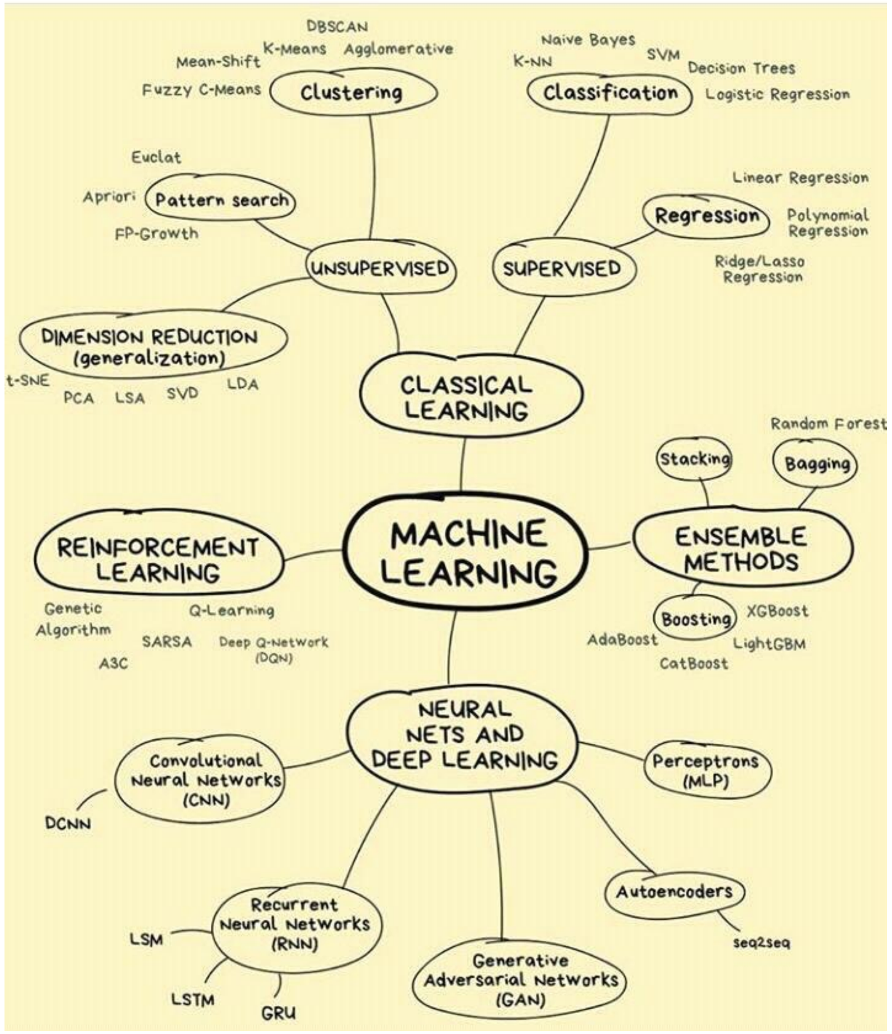
UNSW AUSTRALIA

Recap

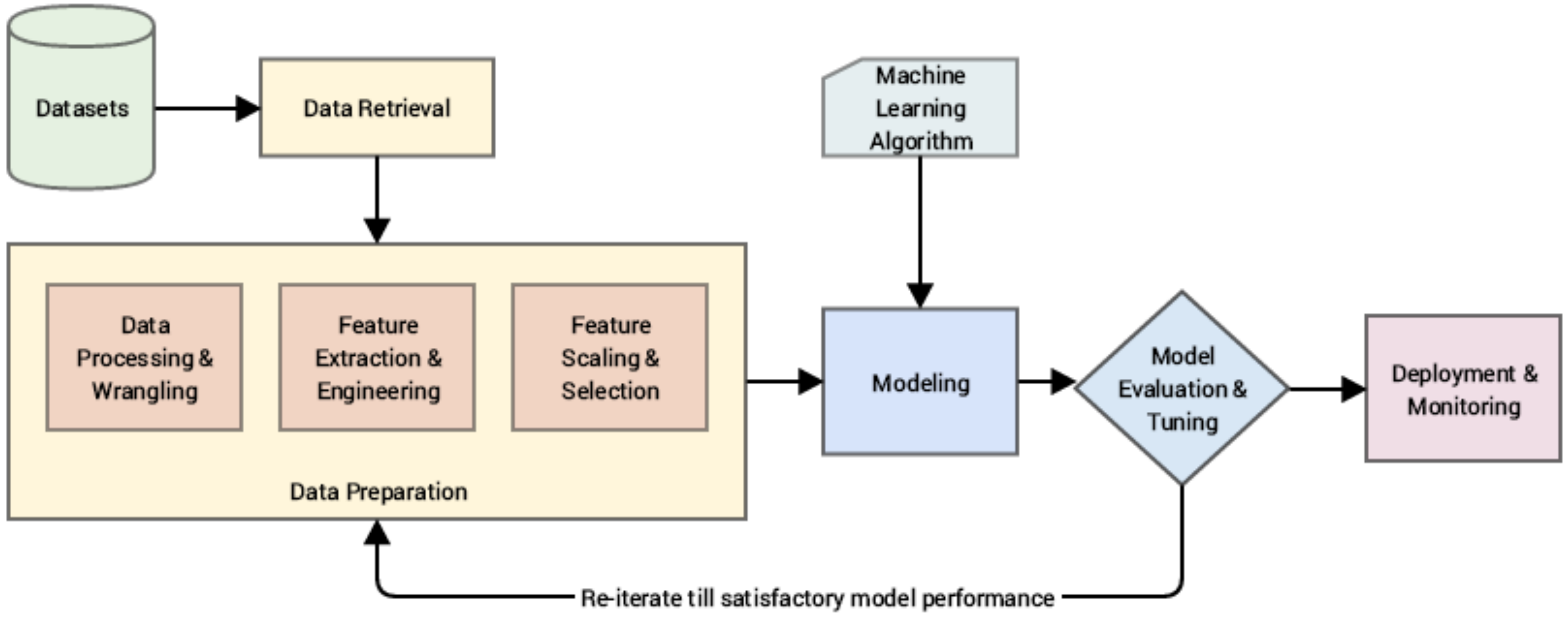
Never Stand Still

COMP9417 Machine Learning & Data Mining

Machine Learning

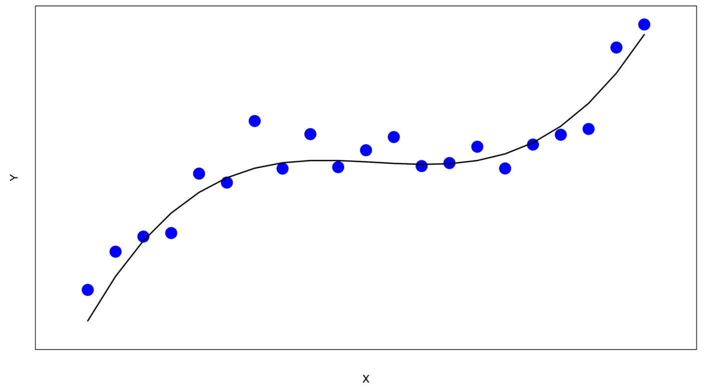


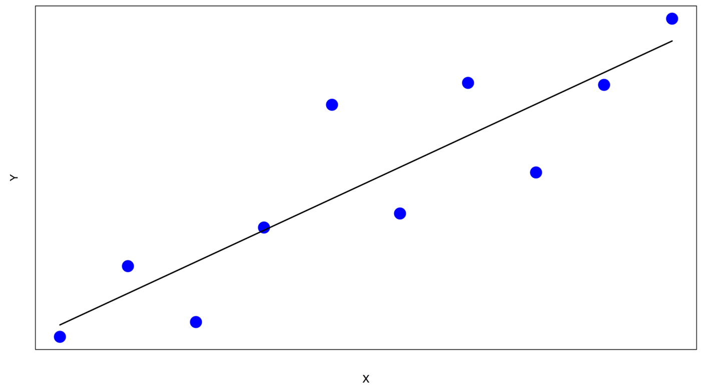
Machine Learning Pipeline


Datasets
Data Retrieval
Machine Learning Algorithm
Data Processing & Wrangling
Feature Extraction & Engineering
Feature Scaling & Selection
Data Preparation
Modeling
Model Evaluation & Tuning
Deployment & Monitoring
Re-iterate till satisfactory model performance

Regression

Regression models are used to predict a continuous value.





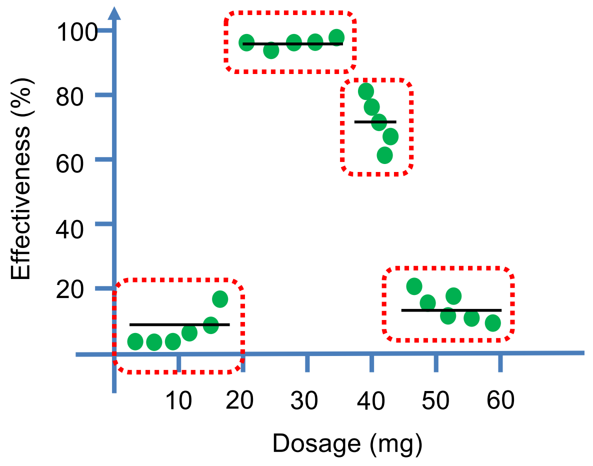
Regression

1. Simple Linear Regression
   - The most common cost function: Mean Squared Error (MSE)
   - Cost function can be minimized using Gradient Descent (it has also closed form solution)
   - Regression coefficients/weights (θ_i) describe the relationship between a predictor variable (x_i) and the output variable (y)
   - Regularization is applied to avoid overfitting
     - It applies additional constrains to the weigh usually to keep weights small (shrinkage) and can be used as feature selection too
     - Most common regularization approaches:
       - Ridge (penalize $\sum_i {\theta_i}^2$)
       - Lasso (penalize $\sum_i |\theta_i|$)
       - Elastic Net (a combination of Ridge and Lasso)

Regression

2. Polynomial Regression
   - Create polynomial terms from your features
   - Will be solved similar to simple Linear Regression
   - Model is still linear in parameters
3. Local regression
   - Use the k nearest neighbors to fit a regression line
   - Produces a piecewise approximation

Regression



4. Decision Tree Regression (regression tree)
   - Partitioning data into homogeneous subsets
   - Variance or standard deviation reduction is used to decide for splitting
   - The predicted value for each leaf is the average value of the samples in that leaf
5. Model Tree
   - Similar to regression trees but with linear regression at each leaf
   - Splitting criterion is standard deviation reduction

Model Evaluation

The most popular metrics are:

- Root Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{m}\sum_{j=1}^{m}(y_j - \hat{y}_j)^2}$$

- Mean Absolute Error (MAE)

$$MAE = \frac{1}{m}\sum_{j=1}^{m}\left|(y_j - \hat{y}_j)\right|$$

- R-squared ($[-\infty, 1]$)

$$R^2 = 1 - \frac{\sum_{j=1}^{m}(y_j - \hat{y}_j)^2}{\sum_{j=1}^{m}(y_j - \bar{y}_j)^2}$$

- Adjuster R-squared

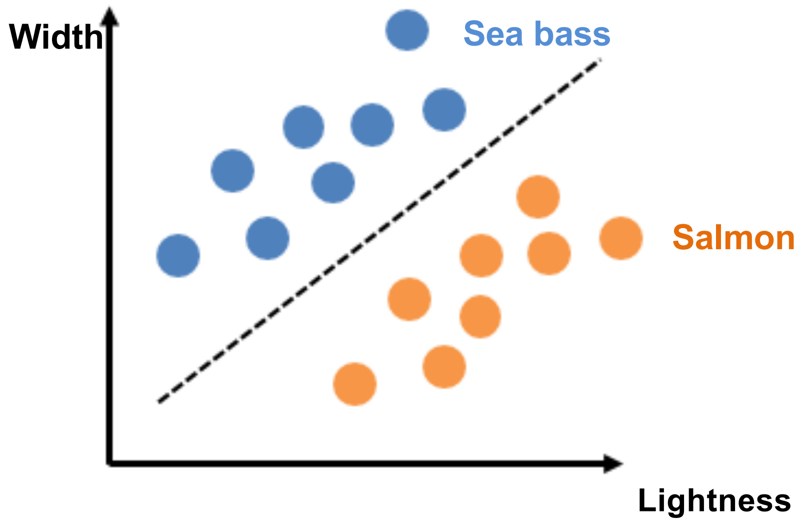
$$R^2_{adjusted} = 1 - [\frac{(1 - R^2)(m - 1)}{m - n - 1}]$$

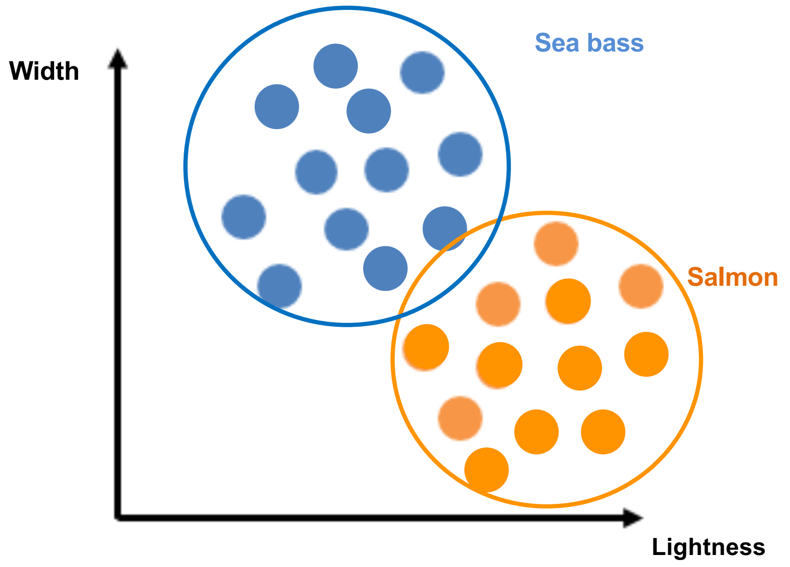
Where m is the total number of samples and n is the number of predictors/features.

- R-squared represents the portion of variance in the output that has been explained by the model

Classification

Classification is prediction of categorical output from input attributes/features.





Classification

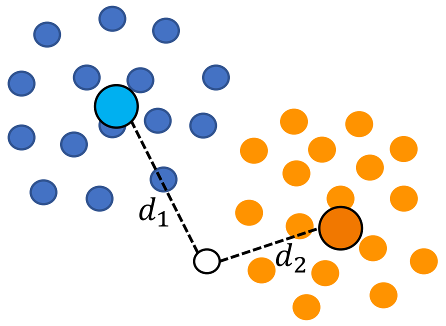
Two main types of classification:

- **Generative algorithm:** builds some models for each of the classes
  - Learns $p(x|y)$
  - and then estimate $p(y|x)$ using Bayes theorem
- **Discriminative algorithm:** Do not build models for different classes, but rather focuses on finding a decision boundary
  - Learns $p(y|x)$ directly

Classification

1. Nearest centroid classifier
   - Distance based classifier
   - $\mu_k = \frac{1}{|C_k|} \sum_{j \in C_k} x_j$
   - For complex classes (eg. Multimodal, non-spherical) may give very poor results
   - Can not handle outliers and noisy data well

   - Not very accurate



Classification

2. k nearest neighbor classifier (kNN)
   - Distance base classifier
   - Find k nearest neighbor using an appropriate distance metric (e.g. Minkowski distance)
   - Predict the output based on the majority vote
   - Works better with lots of training data and small number of attributes
   - Can be very accurate but slow at testing time
   - Curse of dimensionality
   - Assumes all attributes are equally important
     - Remedy: attribute selection or attribute weights
   - Needs homogenous feature type and scale

Classification

3. Bayesian decision theory (based on Bayesian theorem, $P(h|D) = \frac{P(D|h)P(h)}{P(D)}$)
   - The prediction will be the most probable hypothesis if expected loss is equal for all classes :
     - Maximum a posteriori ($h_{MAP} = \arg\max_{h \in H} P(h|D) = \arg\max_{h \in H} P(D|h)P(h)$)
     - If $P(h_i) = P(h_j)$, we use maximum likelihood ($h_{ML} = \arg\max_{h_i \in H} P(D|h_i)$)
   - If the expected loss is not the same, then we have to predict the class which minimizes the expected loss
     - Expected loss: $R(\alpha_i|x) = \sum_{h \in H} \lambda(\alpha_i|h)\ P(h|x)$

Classification

4. Bayes optimal classification: $(\arg\max_{\nu_j \in V} \sum_{h_i \in H} P(\nu_j | h_i) P(h_i | \mathrm{D}))$
   - Here we are dealing with combining the decision from multiple hypothesis
   - No other classification method using the same hypothesis space and same prior knowledge can outperform this method on average
   - Bayes optimal classifier is very inefficient

Classification

5. Naïve Bayes classifier
   - Using Bayesian theory
   - The main difference is the strong assumption that attributes are conditionally independent: $P(x_1, x_2, \ldots, x_n | v_j) = \prod_i P(x_i | v_j)$
   - Prediction is based on maximum a posteriori: $v_{NB} = \arg\max_{v_j \in V} P(x_1, x_2, \ldots, x_n | v_j) \mathrm{P}(v_j) = arg \max_{v_j \in V} \hat{P}(v_j) \prod_i \hat{P}(x_i | v_j)$
   - Useful when:
     - moderate or large training set available
     - Attributes are conditionally independent (however this is usually violated and still NB can do a descent job!)
   - Having too many redundant attributes will decrease the performance

Classification

6. Decision tree:
   - Works in divide and conquer fashion
     - Split into subsets
     - Check the subset purity
       - Use entropy to measure impurity at each node ($E(s) = \sum_{i=1}^{c} -p_i \log_2 p_i$)
       - Use information gain to decide which attribute works better for that node

$$Gain(S, A) = Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

         » However IG is more biased towards attributes with large number of possibilities, so we can use $Gain\ Ratio$ instead
       - Attribute with highest information gain will be selected for the node

Classification

6. Decision tree:
   - Decision trees can work with any type of data (discrete and numeric)
   - Can handle missing values
   - One of the main advantages is interpretability
   - Can almost always classify training example perfectly if we let it grow enough which means it can overfit
   - To avoid overfitting
     - Pre-pruning: stop growing when split is not not statistically significant like chi-squared test(suffer from early stopping). Or limiting $\min\_sample\_leaf$, $\min\_impurity\_decrease$, $\max\_leaf\_node$ or $\max\_depth$, ect.
     - Post-pruning: grow full tree, then remove sub-trees that cause overfitting based on cross validation
   - Greedy algorithm (may not find the optimal tree)

Classification

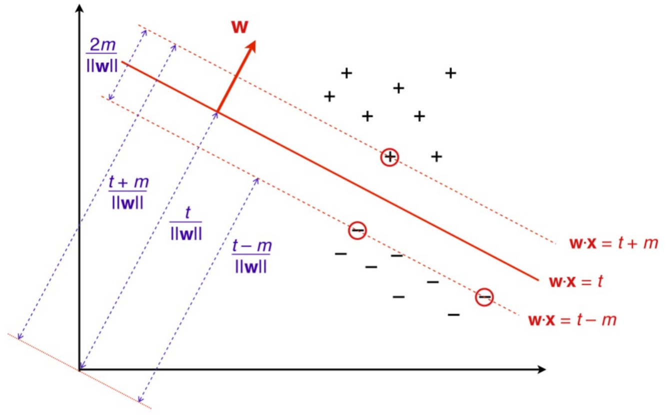
7. Linear Perceptron ($\hat{y} = f(\mathrm{x}) = \mathrm{sgn}(w.\mathrm{x})$)
   - Weights get updated iteratively until no mistake is made or max number of iteration is met
   - Simple and fast at training
   - Doesn't perform well if classes are not linearly separate
8. Non-linear perceptron
   - Map attributes into new space consisting of polynomial terms and interaction terms
   - Use kernel trick to make the computation much less

$$\hat{y} = \mathrm{sign}\left(\sum_{i=1}^{m} \alpha_i y_i (\varphi(\mathrm{x}_i).\varphi(\mathrm{x}))\right)$$

   - A valid kernel function is equivalent to a dot product in some space ($K(\mathrm{x}_i, \mathrm{x}_j) = \varphi(\mathrm{x}_i).\varphi(\mathrm{x}_j)$)

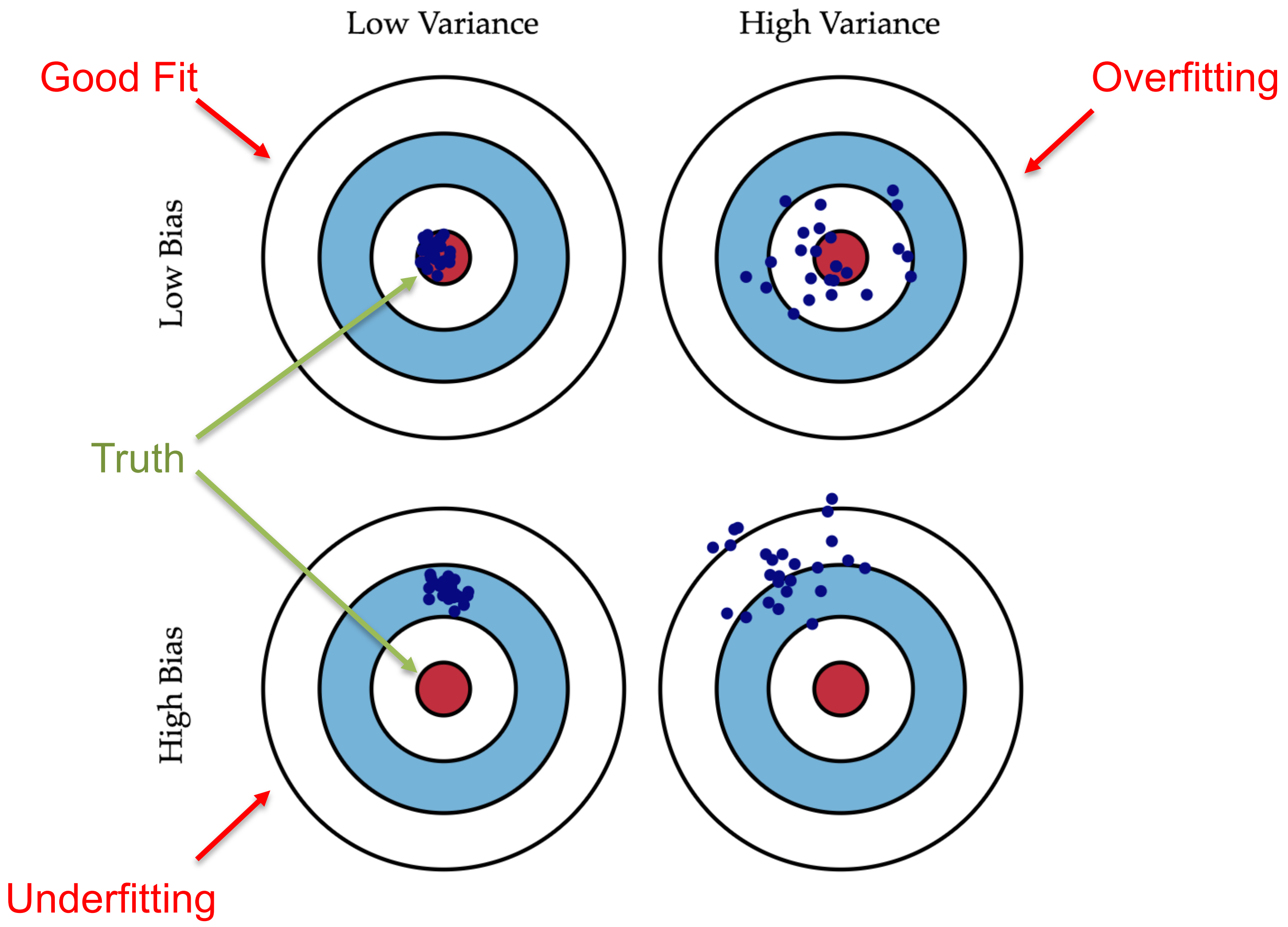
Classification

9. Linear Support Vector Machine (maximum margin)
   - $\hat{y} = sign(\mathrm{w.x} - \mathrm{t})$
   - $w = \sum_{\mathrm{x}_i \in \{support\ vectors\}} \alpha_i y_i x_i$
   - α_i is non-zero for support vectors
   - Is effective in high dimensional data
   - Is effective when number of dimensions is bigger than the number of samples



10. Nonlinear SVM
   - Similar to perceptron, Kernel trick can be applied using dual form
   - $\hat{y} = sign(\sum_{\alpha_i > 0} \alpha_i y_i K(\mathrm{x}_i, \mathrm{x}) - t)$

Bias-Variance Tradeoff



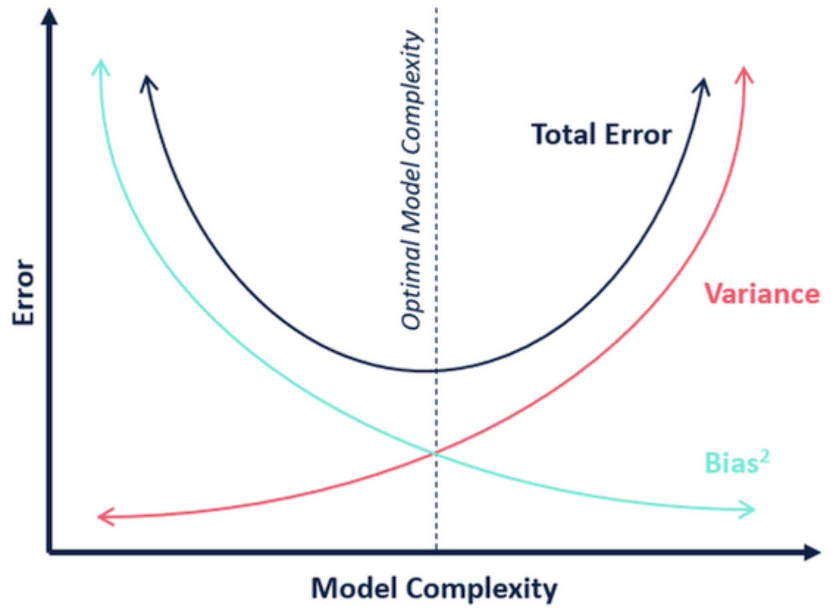
Source: Scott-Fortmann,Understanding Bias-variance tradeoff

Bias-Variance

- Bias-variance:
  - Bias: The inability of the learning algorithm to capture the true relationship between the output and the features/attributes is called **bias**.
    - due to model choice which (e.g. is not complex enough)
  - Variance: The learning algorithm difference in fits between datasets is called **variance**.
    - due to small sample size
    - high complexity of the model

Bias-Variance

- The aim is to have a good bias variance tradeoff
  - methods to find a good bias-variance trade-off:
    - Regularization
    - Ensemble learning in general
    - Bagging
    - Boosting



Ensemble Learning

Ensemble methods: meta-algorithms that combine different models into one model

1. Simple ensembles: combining several learning algorithm
   - Majority vote or unweighted average will be used for prediction
   - Using weighted average or weighted votes to predict the output
   - Treat the output of each algorithm as a feature and train another learning algorithm on them
2. Mixture of experts
   - Each learning algorithm defines $\alpha_i(\mathrm{x})$ which indicated the expertise of that algorithm for that particular location of x in the input space
   - It may use a weighted average or just pick the model with the largest expertise

Ensemble Learning

3. “Bagging” method: (“**B**ootstrap **Agg**regation”)
    - Training many classifiers, but each on a Bootstrapped dataset
        - Bootstrap: Create a random subset of data by sampling with replacement
        - Bagging: Repeat k times to generate k subsets
    - Then aggregate through model averaging / majority voting
    - Bagging is applied on a collection of low-bias high-variance models
        - by averaging them the bias would not get affected
        - by averaging them the variance will be reduced

Ensemble Learning

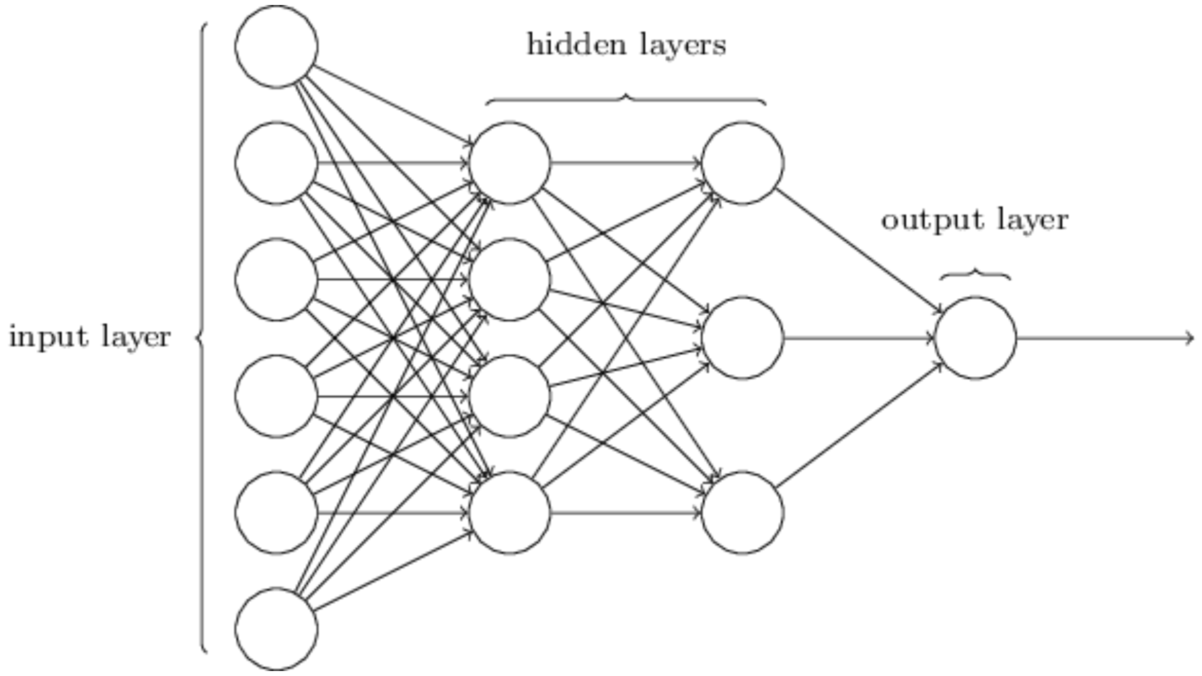
4. Add randomization to the models to introduce more diversity in the models for example
   - For every model use a subset of features, selected randomly, e.g. in Random Forest (it can also help with training time)
   - For algorithms that are dependent on initial weights, use different random initial weights
5. Boosting: A sequence of weak learners, each trying to correct its predecessor
   - Learners are trained sequentially
   - New learners focus on errors of earlier learners
   - New learners try to get misclassified samples right by operating on a weighted training set in favor of misclassified instances
   - Combine all learners in the end using weighted majority/weighted average of k learners

Ensemble Learning

- AdaBoost is a boosting algorithm using stump trees
  - Misclassified instances gain higher weights
  - Correctly classified instances lose weight
- Main advantages:
  - Use very simple (weak) learners
  - It boost the performance
  - Decrease bias
  - Decrease variance
- Slow during training and lack of interpretability
- Gradient Boosting is a boosting algorithm using stump tree for regression
  - At every step models the residuals

Neural Networks

- Neural Nets: composed of a large number of interconnected processing elements known as neurons
  - They use supervised error correcting rules with back-propagation to learn a specific task



Neural Networks

- Perceptron: Output is thresholded sum of products of inputs and their weights
  - Perceptron learning is simply an iterative weight-update ($\mathbf{w}' = \mathbf{w} + \eta y_i \mathbf{x}_i$)
- Multilayer Perceptrons
  - can represent arbitrary functions
  - consists of an input, hidden and output layer each fully connected to the next, with activation feeding forward
- Neural nets are more useful when:
  - Input is high dimensional
  - form of target function is unknown
  - Interpretation is not important

Neural Networks

- Deep Learning: similar to regular neural nets just with more layers
  - Relies on large amount of data
  - Deeper learning architecture
- Convolutional Neural Net: among the most well-known deep learning models
  - Neurons are arranges in 3 dimensions (width, height and depth)
  - Proposes a parameter sharing scheme that minimize the number of parameters
  - Neurons in each layer are only connected to a small region of the layer before it (not fully connected)
  - Parameters of each layer play the role of a filter which is applied locally
  - The pooling layer: to progressively reduce the spatial size of the representation to reduce the number of parameter. Therefore they help with overfitting

Neural Networks

- To avoid overfitting:
  - dropout layer is used
    - In each forward pass, randomly set some neurons to zero
  - Early stopping
  - Reduce the network's capacity by removing some layers
  - Regularisation: adding a cost to the loss function for large weights
  - Data Augmentation
    - Increase the data size
    - Rotation, cropping, scaling, flipping, Gaussina filtering

Evaluation of classification

- For two-class prediction case:

Actual Class	Predicted Class	
	Positive	Negative
Positive	True Positive (TP)	False Negative (FN)
Negative	False Positive (FP)	True Negative (TN)

- $acc = \frac{1}{|Test|} \sum_{x \in Test} I[\hat{c}(X) = c(X)]$
- $Precision = \frac{TP}{TP+FP}$
- $Recall = \frac{TP}{TP+FN}$
- $F_1 = 2.\frac{precision.recall}{precision+recall}$
- $AUC - ROC\ curve$

Missing Values

How to handle missing values (common approaches):

- Deleting samples with missing values
- Replacing the missing value with some statistics from the data (mean, median, …)
- Assigning a unique category
- Predicting the missing values
- Using algorithms that support missing values

Model (Feature) Selection

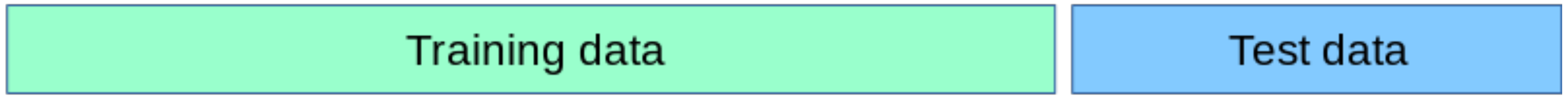
- Taking all the features will lead to an overly complex model. There are 3 ways to reduce complexity:
  - Subset-selection: feature forward selection, feature backward selection or feature importance analysis
  - Shrinkage, or regularization of coefficients to zero, by optimization. There is a single model, and unimportant variables have near-zero coefficients.
  - Dimensionality-reduction, by projecting points into a lower dimensional space

Data Normalization

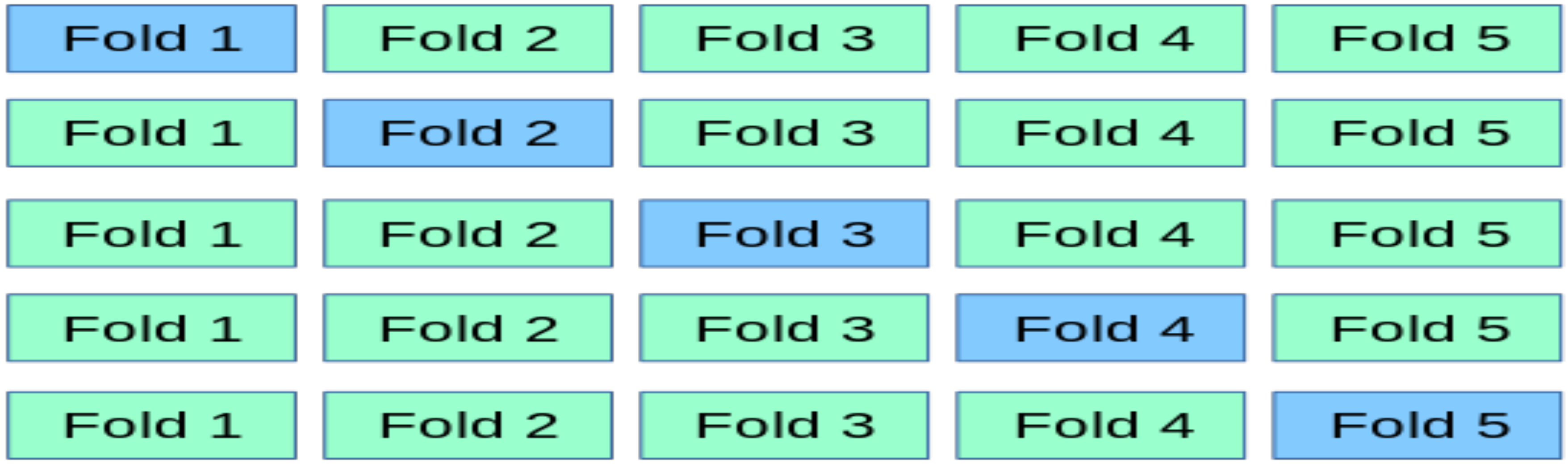
- Normalization is usually a data pre-processing step that change the values of numeric columns in the dataset to a common scale, without distorting differences in the ranges of values.
  - Most of the distance based machine learning algorithms require normalization as a processing step if features do not have same scales
  - Most common normalization techniques:
    - Min-max normalization: $x' = \frac{x - \min(x)}{\max(x) - \min(x)}$
    - Z-score (standardization):$x' = \frac{x - \bar{x}}{\sigma}$

Validation

- Hold-out method:



- K-fold cross validation



Unsupervised Learning

Unsupervised learning: classes are initially *unknown* and need to be "discovered" with their definitions from the data

- It is useful for:
  - Dimensionality reduction (simplify the problem, getting rid of redundant feature)
  - exploratory data analysis
  - to group data instances into subsets
  - to discover structure, like hierarchies of subconcepts
  - to learn new "features" for later use in classification
  - to track "concept drift" over time

Clustering

- Goal: form homogeneous cluster and well separated clusters
- Success of clustering often measured subjectively
- There are two broad types of clustering:
  - Hierarchical methods
  - Partitioning methods

Clustering

1. K-means
   - Initialize k random centers from the data
   - Assign each instance to the closest center and re-compute the centers using mean or weighted average and re-iterate
   - Simple and can be efficient clustering method
   - Not easy to predict k
   - Different initialization can result different clusters
   - Sensitive to outliers

Clustering

2. Expectation Maximization:
   - Similar to k-means
   - Computes probabilities of cluster memberships based on one or more probability distributions. (e.g. mixture of Gaussian)
   - The goal is to maximize the overall probability or likelihood of the data, given the (final) clusters.
   - Easy with independence assumption

Clustering

3. Hierarchical clustering
   - Agglomerative :starts by treating each object as a singleton cluster and gradually merge based on similarity
   - Divisive: it starts by including all objects in a single large cluster. At each step of iteration, the most heterogeneous cluster is divided into two. The process is iterated until all objects are in their own cluster.
   - Do not require to specify the number of clusters
   - Different linkage methods can produce very different dendrograms

Clustering

- Finding number of clusters:
  - Elbow method: using the within-cluster dispersion
  - Gap statistics: based on the within-cluster variance of original data and B sets of resampled data
    - Choose the number of clusters as the smallest value of k such that the gap statistic is within one standard deviation of the gap at k+1
- Quality of clusters
  - if clusters known, measure proportion of disagreements to agreements
  - if unknown, measure homogeneity and separation
  - silhouette method

Dimensionality Reduction

- Dimensionality reduction: is the process of reducing the number of feature/attributes
  - Helps with removing redundant/correlated feature
  - Helps with curse of dimensionality

1. Principal Component Analysis (PCA): to capture the direction of the most variation in the original data space.
   - Features are not correlated in the new space (they are orthogonal)
   - New dimensions are computed using eigenvectors and eigenvalues of the data matrix (rows are observations and columns are features)
   - Note: Feature have to be normalized before applying PCA
2. Autoencoders: A neural network model – the encoder transforms the data into smaller dimension such that the decoder can then interpret and reconstruct with minimum error