HANDS-ON AI I

Supervised Machine Learning Basics

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Copyright Statement

Content of Unit 3

- Introduction to machine learning
- Some machine learning algorithms

INTRODUCTION TO MACHINE LEARNING

How to Solve These Tasks?

- Prediction of trajectory of a space shuttle
- Translation of one language into another
- Prediction of protein function
- Automatic recognition of handwritten digits
- Object detection in images

Explicit Models

Traditional approach: **Explicit model**

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- Use explicit knowledge to design model **deductively**.
- Pros:
  - Knowledge about behavior of model and environment/problem.
  - Knowledge about restrictions of model and reasons for design choices.
- Cons:
  - Sometimes problem is too complex to model.
  - Consequences of simplifications of problem/model hard to assess.
  - Insufficient knowledge about problem/environment.

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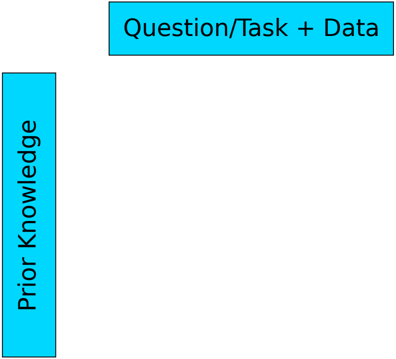
- **Classification**: target value is class label
- **Regression**: target value is numerical value

Terminology

- **Model**: parameterized function/method with specific parameter values (e.g., a trained neural network)
- **Model class**: the class of models in which we search for the model (e.g., neural networks, SVMs, ...)
- **Parameters**: what is adjusted during training (e.g., network weights)
- **Hyperparameters**: settings controlling model complexity or the training procedure (e.g., network learning rate)
- **Model selection/training**: process of finding a model (optimal parameters) from the model class

Basic Data Analysis Workflow



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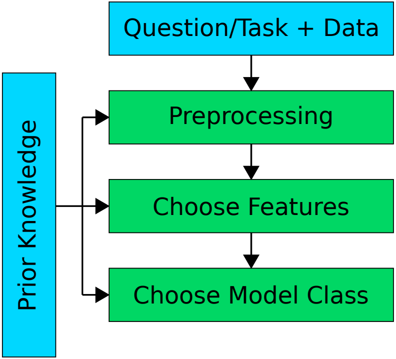

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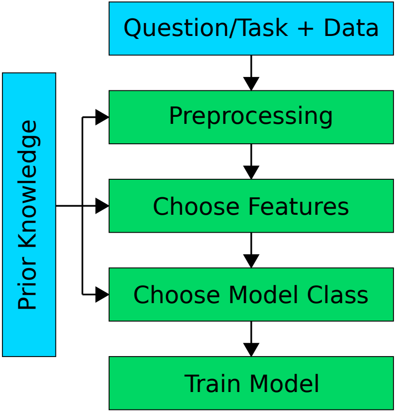

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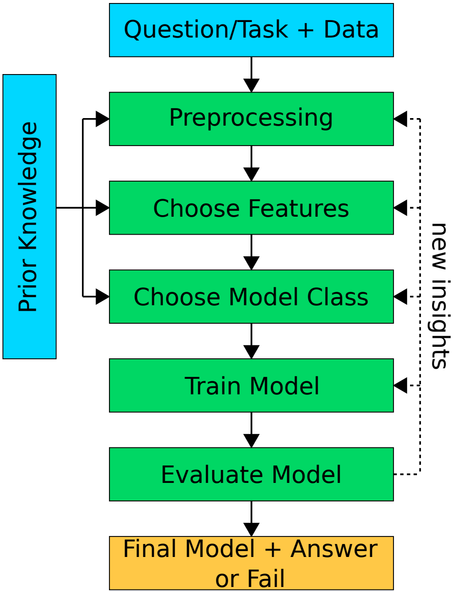

Introductory Example: Fish Recognition

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$\rightarrow$ **Classification** task with two labels (salmon vs. sea bass, or, alternatively, salmon vs. not salmon)

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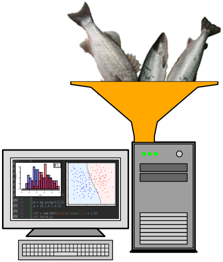

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How can we distinguish these two kinds of fish?

First step: Let's take a look at our data!

Feature Selection & Preprocessing

- **Feature selection**:
  - What data do we have?
  - Removal of redundant features.
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- **Preprocessing**:
  - Contrast and brightness correction
  - Segmentation
  - Alignment
  - Normalization
  - ...

Back to Our Data

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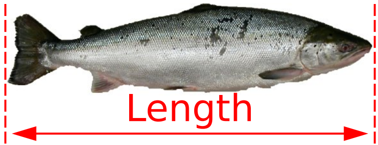

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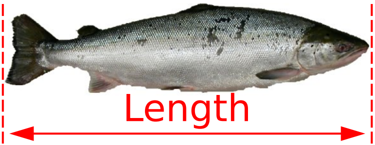

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$\rightarrow$ How do we express/represent these features?

Input Representation

- We can represent an object by a vector $\boldsymbol{x}$ of feature values (=**feature vector**) of length d and **label** y:

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- An object described by one feature vector and one label is referred to as **sample**: $(\boldsymbol{x}, y)$.

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$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_n \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

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- Our labeled data is thus described by: $(\boldsymbol{X}, \boldsymbol{y})$.

Back to Our Data

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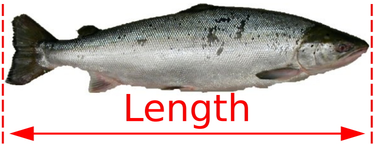
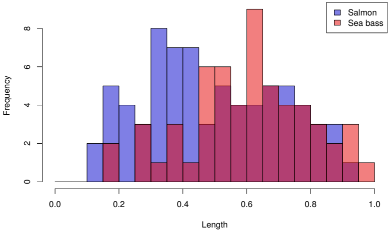


Sea bass:

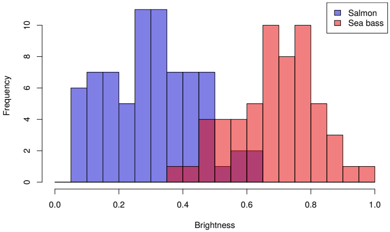
- We now know how to represent our data (i.e., using **features** and **labels**) and will take a look at it via histograms.

Back to Our Data

Length:



Brightness:



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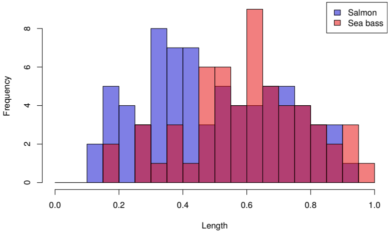

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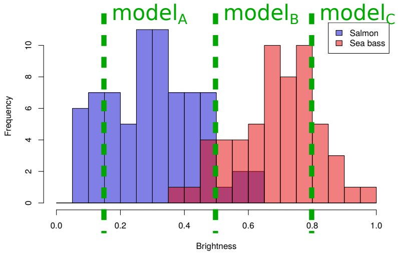

- Brightness looks more useful for fish classification.
- 3 different models based on brightness threshold:
  - model_A: brightness $< 0.18 \rightarrow$ Salmon
  - model_B: brightness $< 0.5 \rightarrow$ Salmon
  - model_C: brightness $< 0.8 \rightarrow$ Salmon

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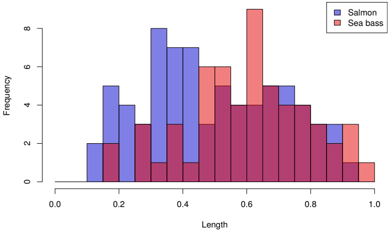

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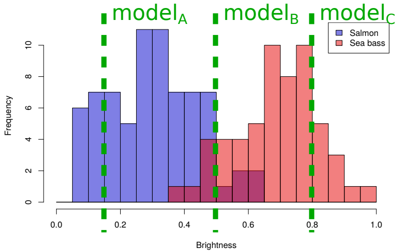

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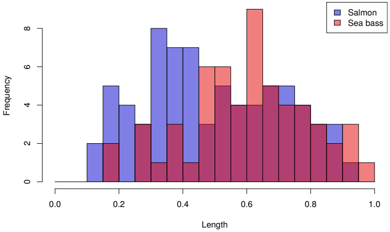

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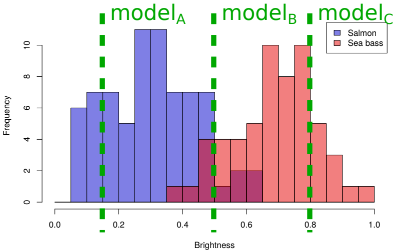

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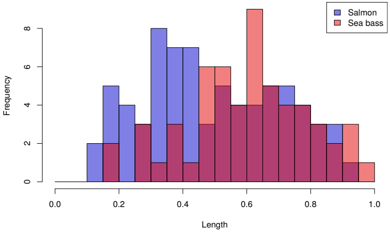

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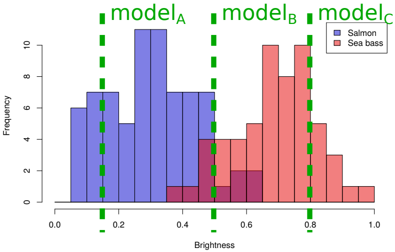

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LOSS FUNCTION

Scoring Our Models: Loss Function

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- **The smaller the loss/cost, the better our prediction**.

Examples of Loss Functions

Zero-one loss: $L_{\mathbf{zo}}(y, g(\boldsymbol{x}; \boldsymbol{w})) = \begin{cases} 0 & y = g(\boldsymbol{x}; \boldsymbol{w}) \\ 1 & y \neq g(\boldsymbol{x}; \boldsymbol{w}) \end{cases}$

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- Many other loss functions available with different justifications.
- Not every loss function is suitable for every task.
- Choice of loss function depends on data, task, and model class.

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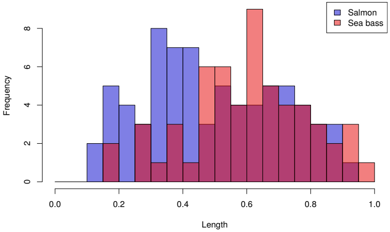

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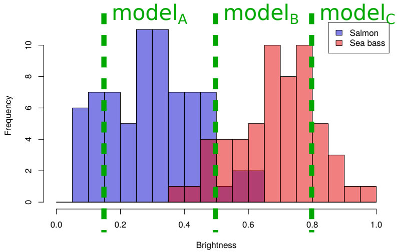

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GENERALIZATION ERROR/RISK

Generalization Error/Risk

- The **generalization error** or **risk** is the expected loss on future data for a given model $g(.;\boldsymbol{w})$:

$$R(g(.;\boldsymbol{w})) = \int_{\boldsymbol{X}} \int L(y, g(\boldsymbol{x};\boldsymbol{w})) \cdot p(\boldsymbol{x}, y) dy d\boldsymbol{x}$$

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$\rightarrow$ We have to **estimate the generalization error**:

- This is called **empirical risk minimization (ERM)**

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- Law of large numbers:

$$R_E(g(.;\boldsymbol{w})) \rightarrow R(g(.;\boldsymbol{w})) \quad \text{for } n \rightarrow \infty$$

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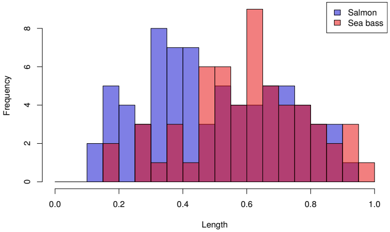

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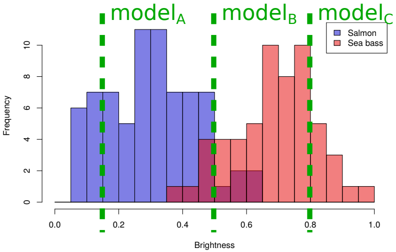

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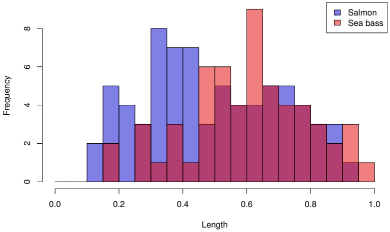

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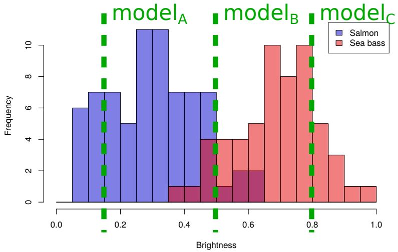

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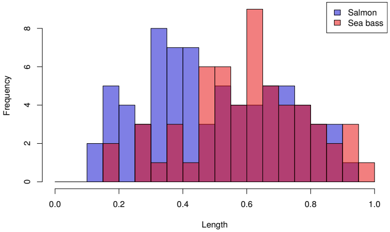

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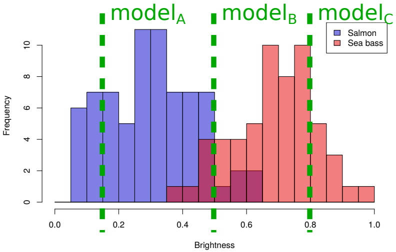

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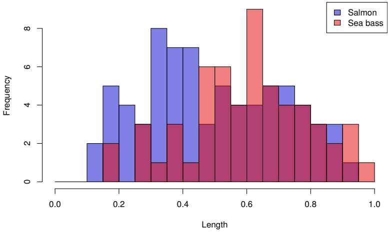

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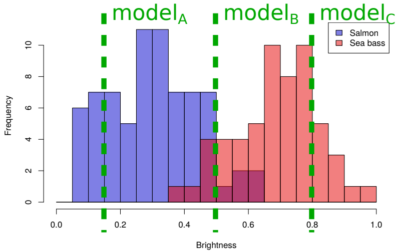

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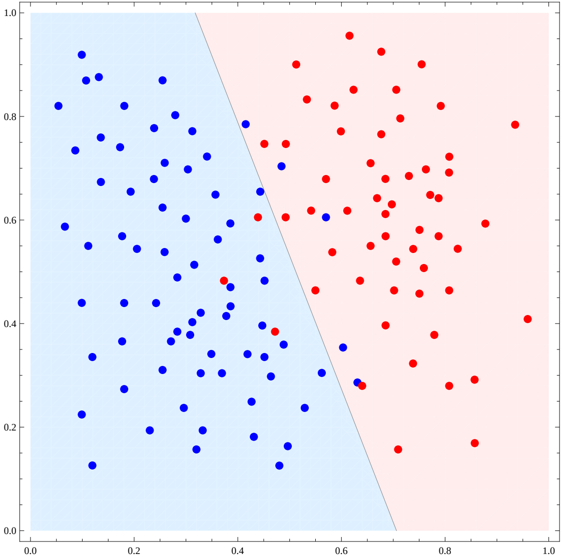
$\rightarrow$ **Combine our features** and use a different model class.

Combination: Linear Separation



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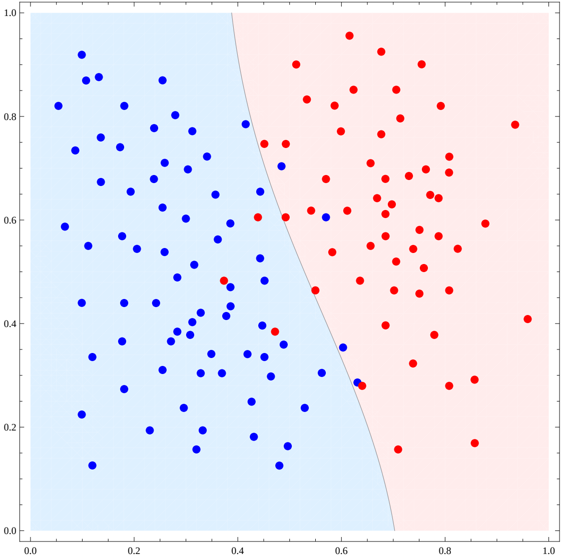
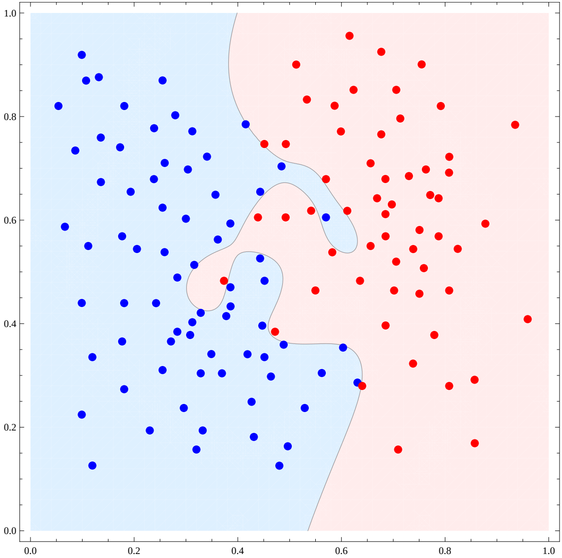
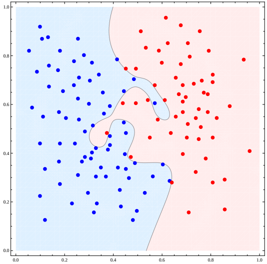


Combination: Highly Non-linear Separation



The Problem of Overfitting



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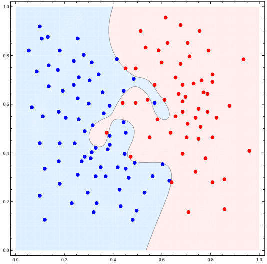

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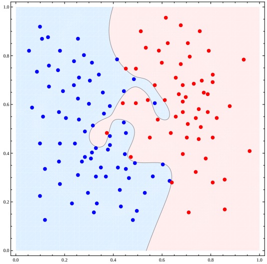

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$\rightarrow$ We need to get a better estimate for the (true) risk.

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- Our estimate R_E on the test set will show if we overfit to noise in the training set.

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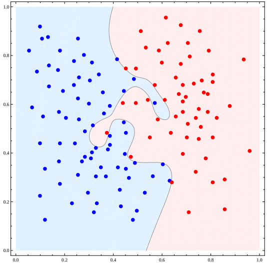

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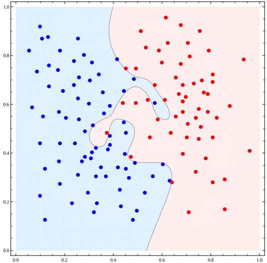

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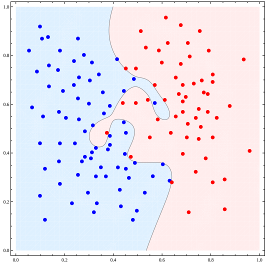

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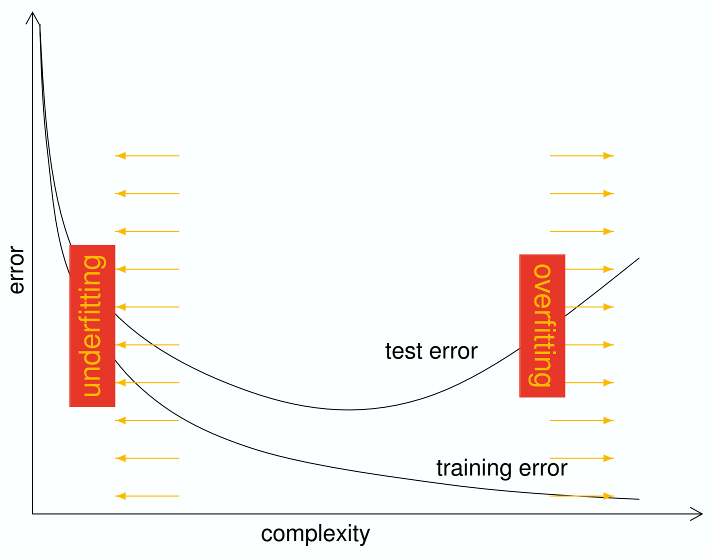

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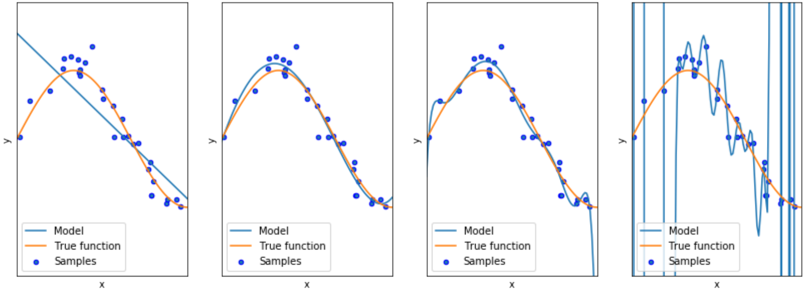

SOME MACHINE LEARNING ALGORITHMS

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- We now look more closely at three different machine learning algorithms:
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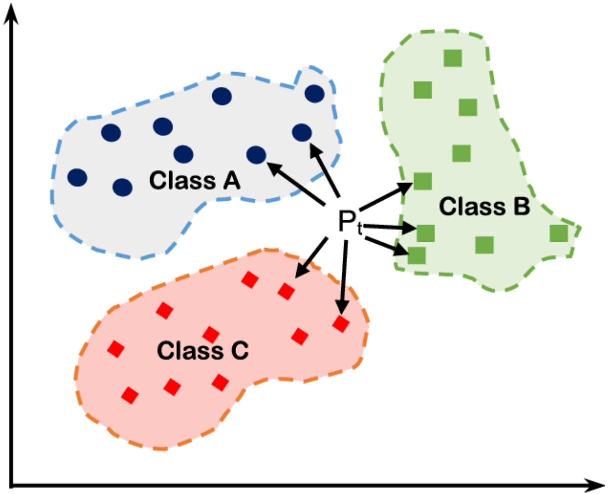
- This should provide a rough idea on the diversity of ideas and algorithms on the market.
- A profound mathematical treatment of the algorithms is given, e.g., in **Machine Learning: Supervised Techniques**.

k-Nearest Neighbors Classifier



Picture taken from: https://www.researchgate.net/publication/331424423

k-Nearest Neighbors Classifier (1)

- Assume we have a labeled data set $(\boldsymbol{X}, y)$ and a **distance measure on the input space**. Then the **k-nearest neighbors classifier** is defined as follows:

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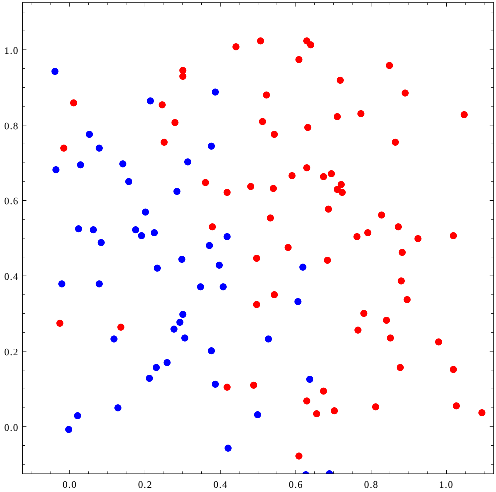
- In case of ties: e.g., random class assignment or class with larger number of samples is assigned.

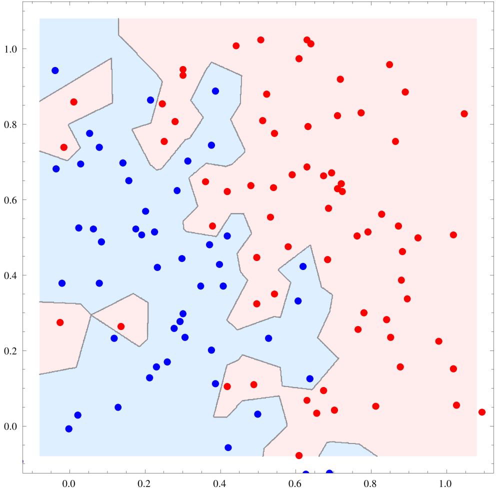
k-Nearest Neighbors Classifier (2)

Input data set



k-Nearest Neighbors Classifier (3)

$k = 1$



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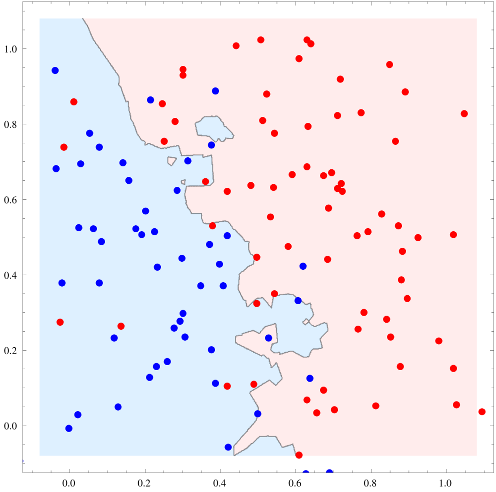
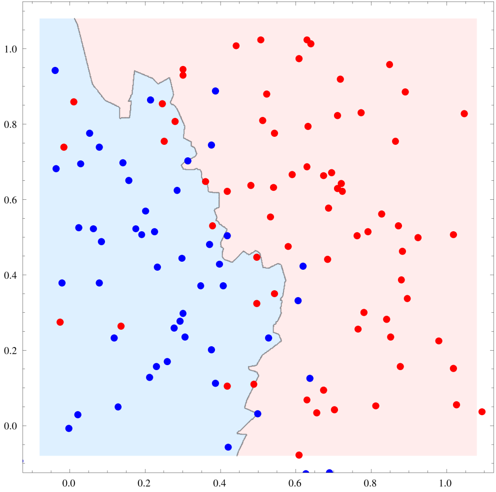


k-Nearest Neighbors Classifier (5)

$k = 13$



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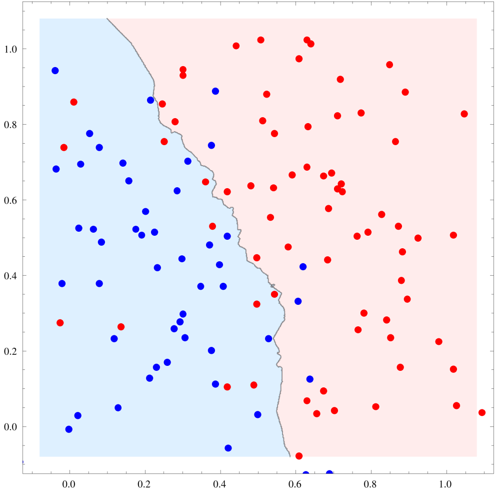
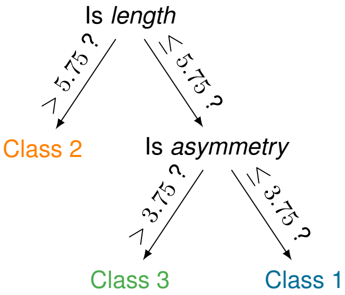
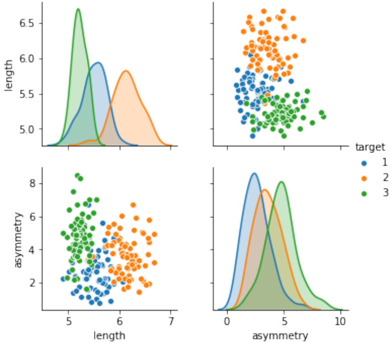


Decision Trees





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- Two famous algorithms use decision trees:
  - Random forest
  - Gradient boosting

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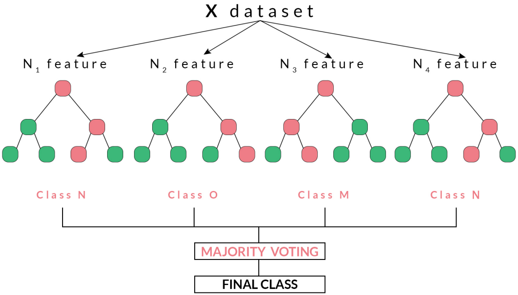

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