# Artificial Intelligence for Medicine II

Spring 2025

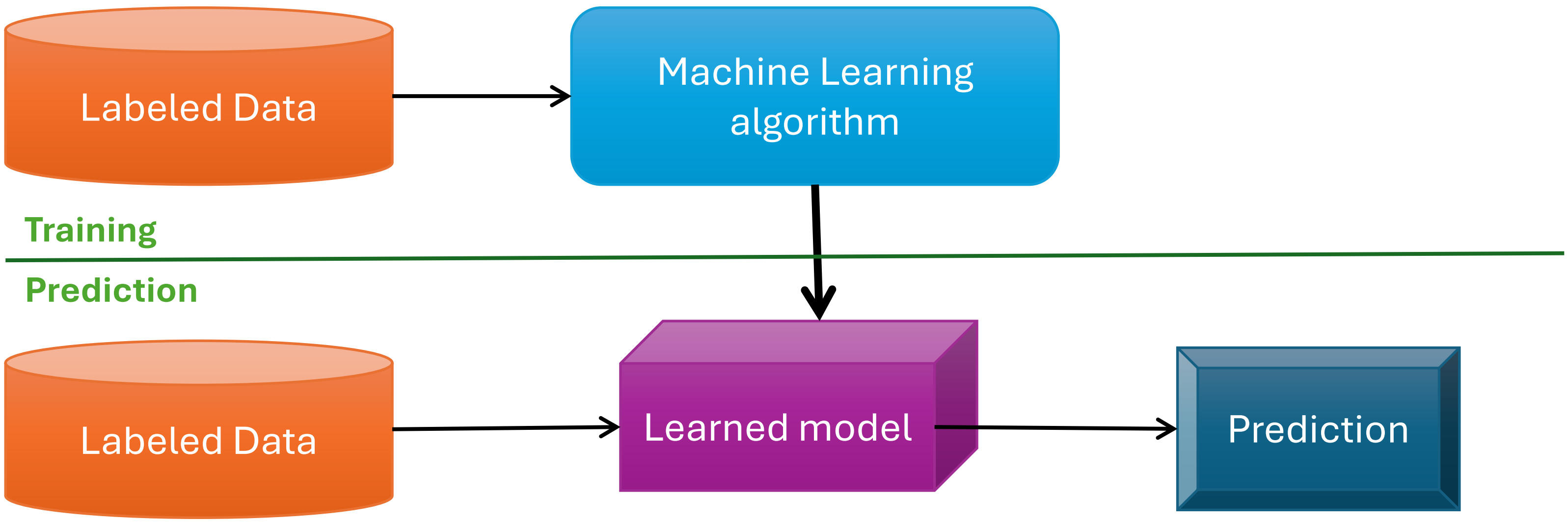
**Lecture 111: Machine Learning Overview**

(Many slides adapted from mostly Alex Vakanski, D. Jurafsky, Bing Liu, Han, Kamber & Pei; Tan, Steinbach, Kumar and the web)

# Machine Learning Basics



- ***Artificial Intelligence*** is a scientific field concerned with the development of algorithms that allow computers to learn without being explicitly programmed
- ***Machine Learning*** is a branch of Artificial Intelligence, which focuses on methods that learn from data and make predictions on unseen data

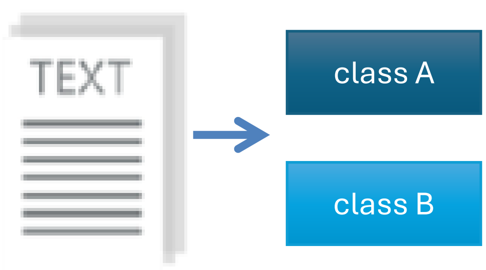



Picture from: Ismini Lourentzou – Introduction to Deep Learning

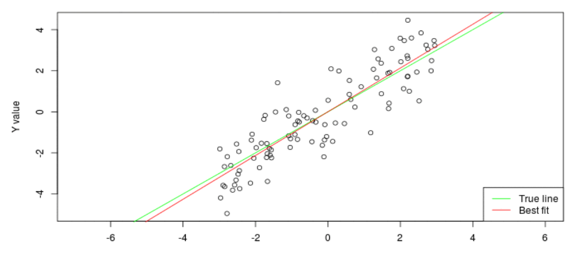
# Machine Learning Types

*Machine Learning Basics*

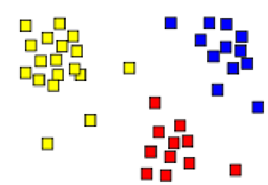
- ***Supervised***: learning with labeled data
  - Example: email classification, image classification
  - Example: regression for predicting real-valued outputs
- ***Unsupervised***: discover patterns in unlabeled data
  - Example: cluster similar data points
- ***Reinforcement learning***: learn to act based on feedback/reward
  - Example: learn to play Go




Classification




Regression



Clustering

# Supervised Learning



- *Supervised learning* categories and techniques
  - **Numerical classifier functions**
    - Linear classifier, perceptron, logistic regression, support vector machines (SVM), neural networks
  - **Parametric (probabilistic) functions**
    - Naïve Bayes, Gaussian discriminant analysis (GDA), hidden Markov models (HMM), probabilistic graphical models
  - **Non-parametric (instance-based) functions**
    - $k$-nearest neighbors, kernel regression, kernel density estimation, local regression
  - **Symbolic functions**
    - Decision trees, classification and regression trees (CART)
  - **Aggregation (ensemble) learning**
    - Bagging, boosting (Adaboost), random forest

Slide credit: Y-Fan Chang – An Overview of Machine Learning

# Unsupervised Learning

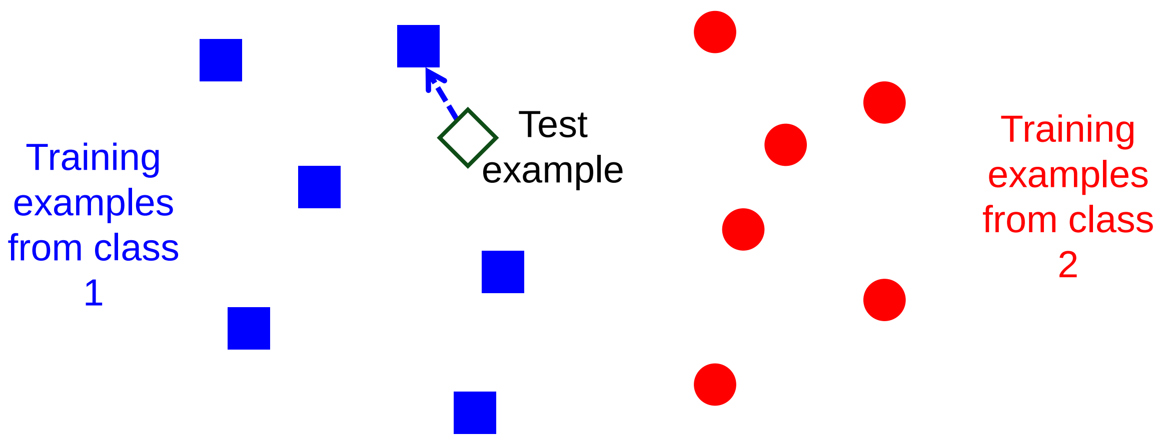


- ***Unsupervised learning*** categories and techniques
  - **Clustering**
    - *k*-means clustering
    - Mean-shift clustering
    - Spectral clustering
  - **Density estimation**
    - Gaussian mixture model (GMM)
    - Graphical models
  - **Dimensionality reduction**
    - Principal component analysis (PCA)
    - Factor analysis

# Nearest Neighbor Classifier



- ***Nearest Neighbor*** – for each test data point, assign the class label of the nearest training data point
  - Adopt a distance function to find the nearest neighbor
    - Calculate the distance to each data point in the training set, and assign the class of the nearest data point (minimum distance)
  - It does not require learning a set of weights

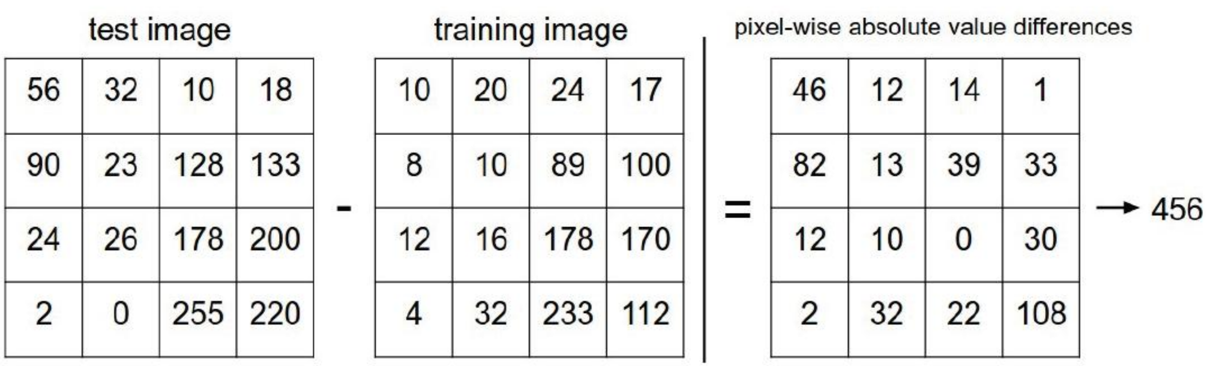



Picture from: James Hays – Machine Learning Overview

# Nearest Neighbor Classifier



- For image classification, the distance between all pixels is calculated (e.g., using $\ell_1$ norm, or $\ell_2$ norm)
  - Accuracy on CIFAR-10: 38.6%
- Disadvantages:
  - The classifier must remember all training data and store it for future comparisons with the test data
  - Classifying a test image is expensive since it requires a comparison to all training images




$\ell_1$ norm
(Manhattan distance)

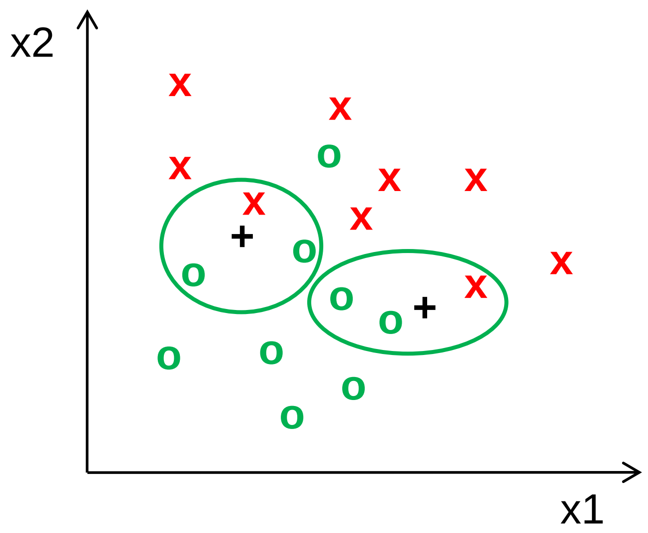
$$d_1(I_1, I_2) = \Sigma_p \, |I_1^p - I_2^p|$$

Picture from: https://cs231n.github.io/classification/

# *k*-Nearest Neighbors Classifier



- ***k-Nearest Neighbors*** approach considers multiple neighboring data points to classify a test data point
  - E.g., 3-nearest neighbors
    - The test example in the figure is the + mark
    - The class of the test example is obtained by voting (based on the distance to the 3 closest points)




Picture from: James Hays – Machine Learning Overview

# Linear Classifier



- ***Linear classifier***
  - Find a linear function $f$ of the inputs $x_i$ that separates the classes

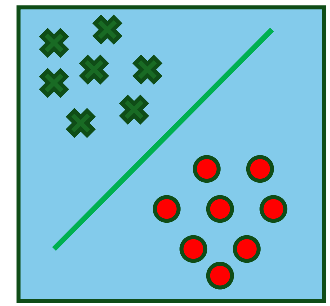
$$f(x_i, W, b) = Wx_i + b$$

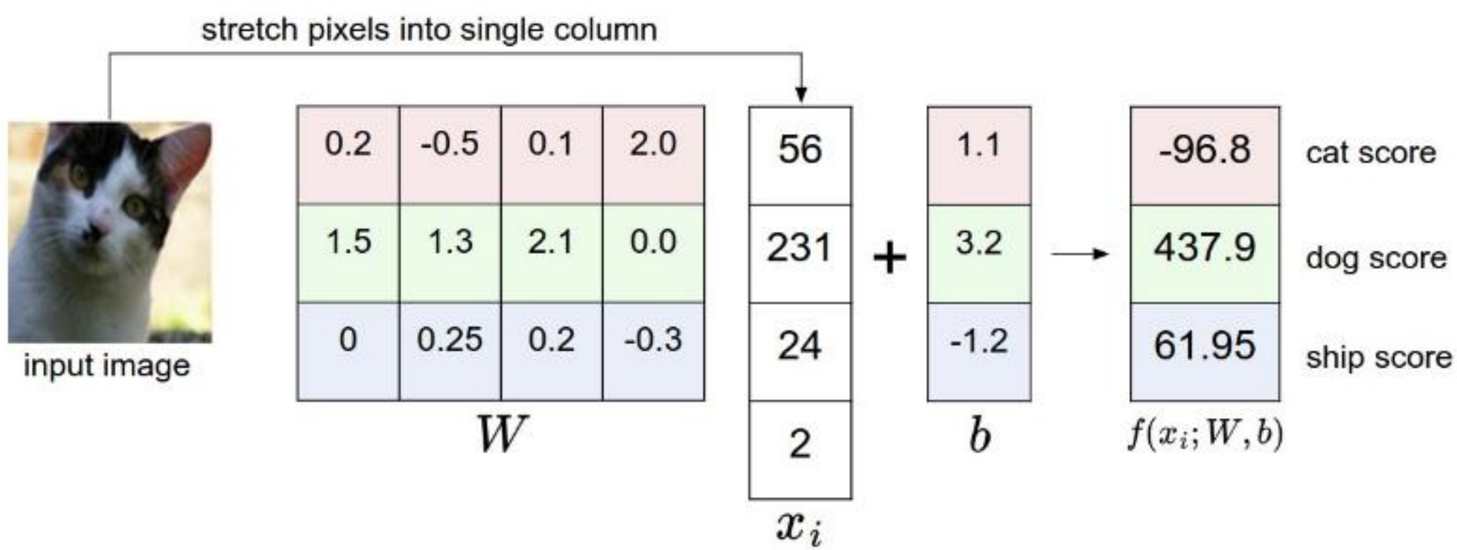
  - Use pairs of inputs and labels to find the weights matrix $W$ and the bias vector $b$
    - The weights and biases are the parameters of the function $f$
  - Several methods have been used to find the optimal set of parameters of a linear classifier
    - A common method of choice is the ***Perceptron*** algorithm, where the parameters are updated until a minimal error is reached (single layer, does not use backpropagation)
  - Linear classifier is a simple approach, but it is a building block of advanced classification algorithms, such as SVM and neural networks
    - Earlier multi-layer neural networks were referred to as multi-layer perceptrons (MLPs)

# Linear Classifier



- The decision boundary is linear
  - A straight line in 2D, a flat plane in 3D, a hyperplane in 3D and higher dimensional space
- Example: classify an input image
  - The selected parameters in this example are not good, because the predicted cat score is low






Picture from: https://cs231n.github.io/classification/

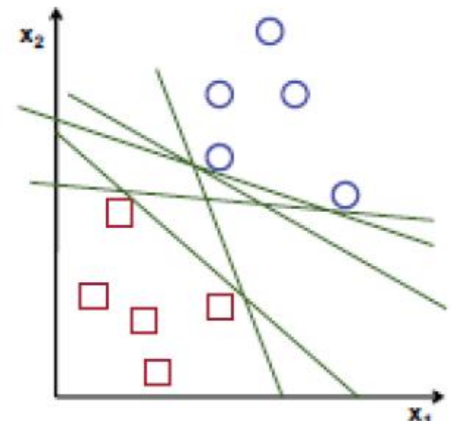
# Support Vector Machines

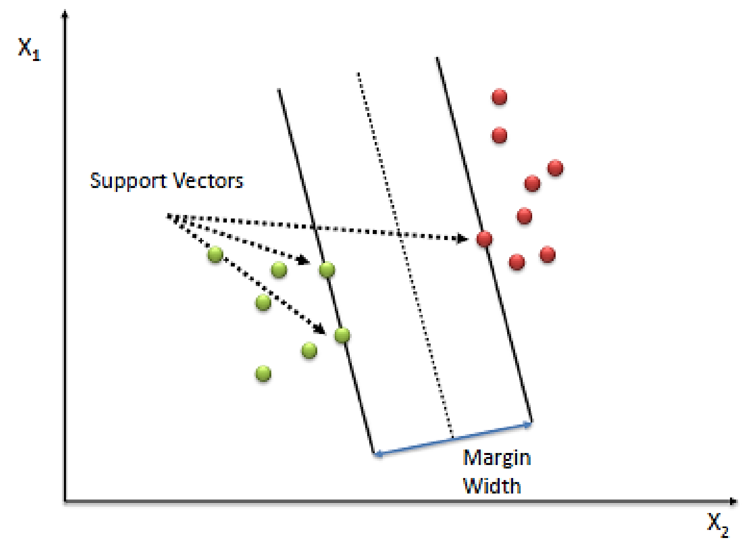


- ***Support vector machines (SVM)***
  - How to find the best decision boundary?
    - All lines in the figure correctly separate the 2 classes
    - The line that is farthest from all training examples will have better generalization capabilities
  - SVM solves an optimization problem:
    - First, identify a decision boundary that correctly classifies the examples
    - Next, increase the geometric margin between the boundary and all examples
  - The data points that define the maximum margin width are called support vectors
  - Find $W$ and $b$ by solving:

$$\min \frac{1}{2}\|w\|^2$$

$$s.t.\ y_i(w \cdot x_i + b) \geq 1,\ \forall x_i$$



# Linear vs Non-linear Techniques

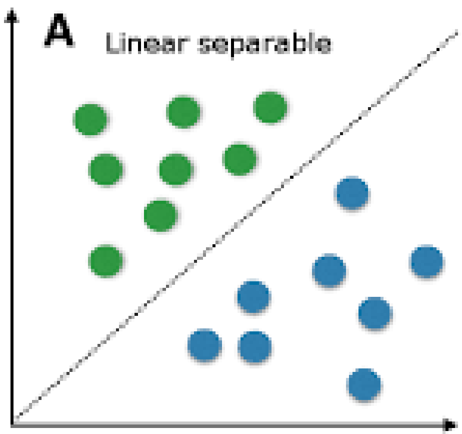


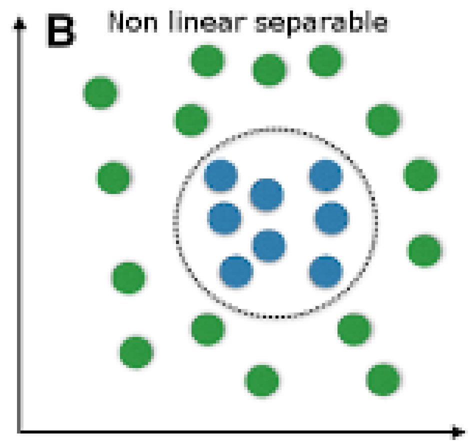
- Linear classification techniques
  - Linear classifier
  - Perceptron
  - Logistic regression
  - Linear SVM
  - Naïve Bayes
- Non-linear classification techniques
  - *k*-nearest neighbors
  - Non-linear SVM
  - Neural networks
  - Decision trees
  - Random forest

# Linear vs Non-linear Techniques

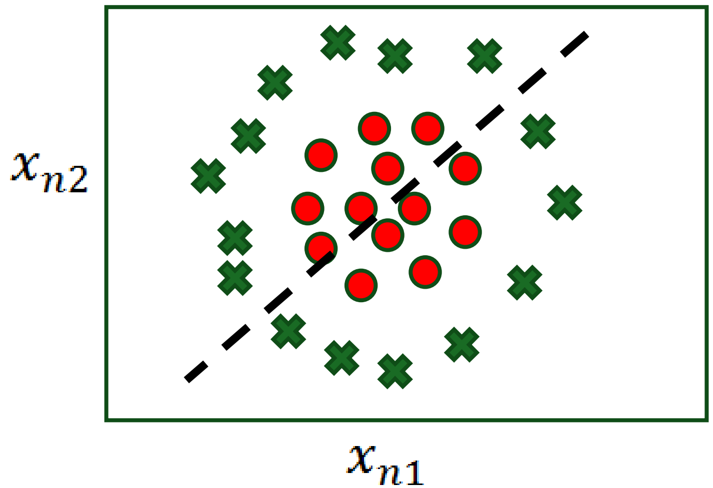


- For some tasks, input data can be linearly separable, and linear classifiers can be suitably applied




- For other tasks, linear classifiers may have difficulties to produce adequate decision boundaries

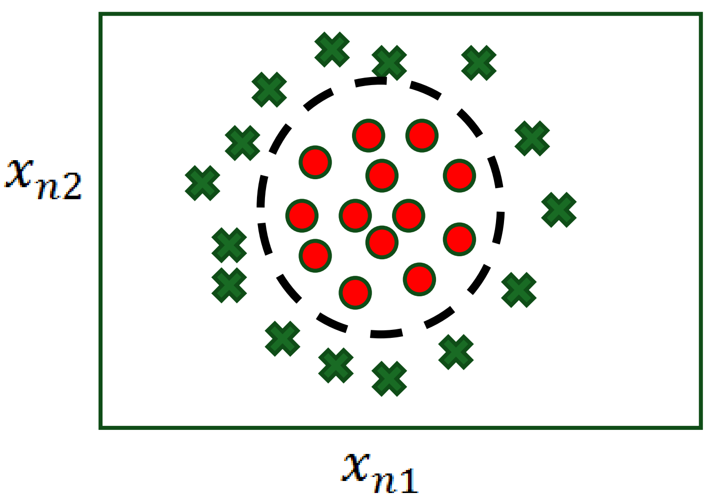



Picture from: Y-Fan Chang – An Overview of Machine Learning

# Non-linear Techniques

*Linear vs Non-linear Techniques*

- Non-linear classification
  - Features $z_i$ are obtained as non-linear functions of the inputs $x_i$
  - It results in non-linear decision boundaries
  - Can deal with non-linearly separable data




Inputs: $x_i = [x_{n1} \quad x_{n2}]$

Features: $z_i = [x_{n1} \quad x_{n2} \quad x_{n1} \cdot x_{n2} \quad x_{n1}^2 \quad x_{n2}^2]$

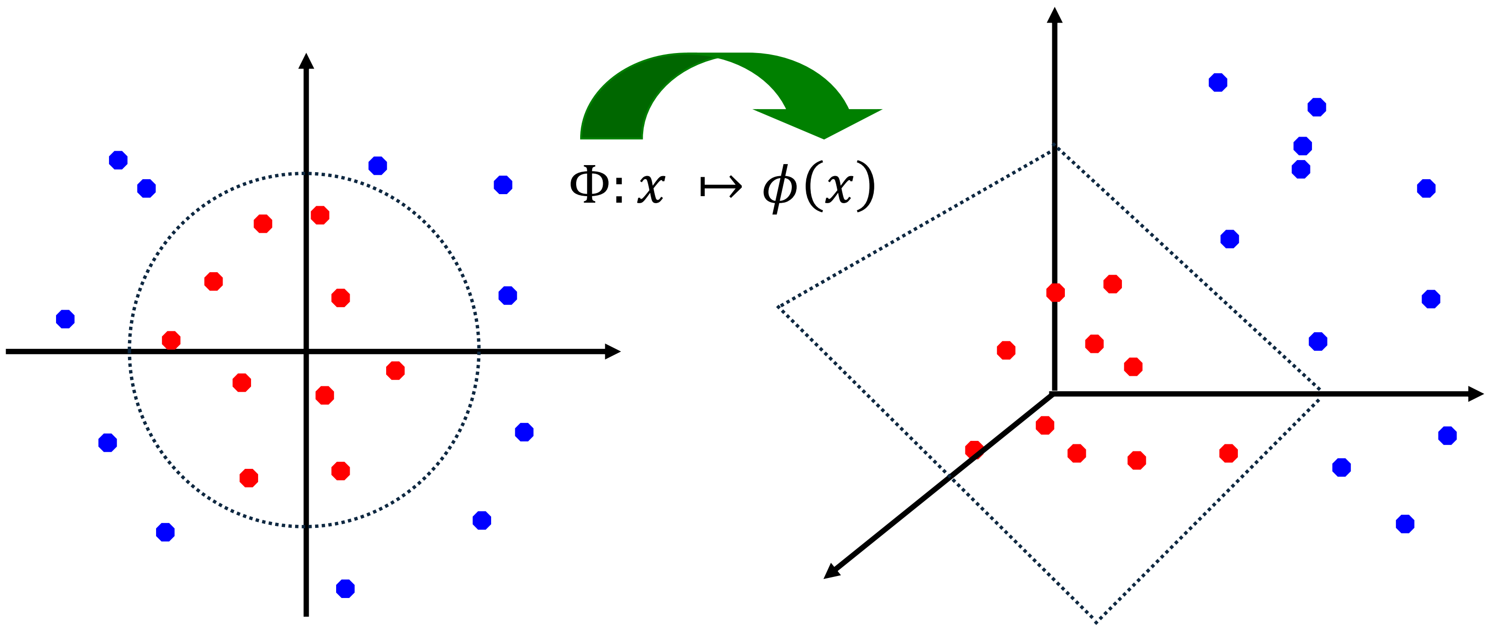
Outputs: $f(x_i, W, b) = W z_i + b$

Picture from: Y-Fan Chang – An Overview of Machine Learning

# Non-linear Support Vector Machines

*Linear vs Non-linear Techniques*

- ***Non-linear SVM***
  - The original input space is mapped to a higher-dimensional feature space where the training set is linearly separable
  - Define a non-linear kernel function to calculate a non-linear decision boundary in the original feature space

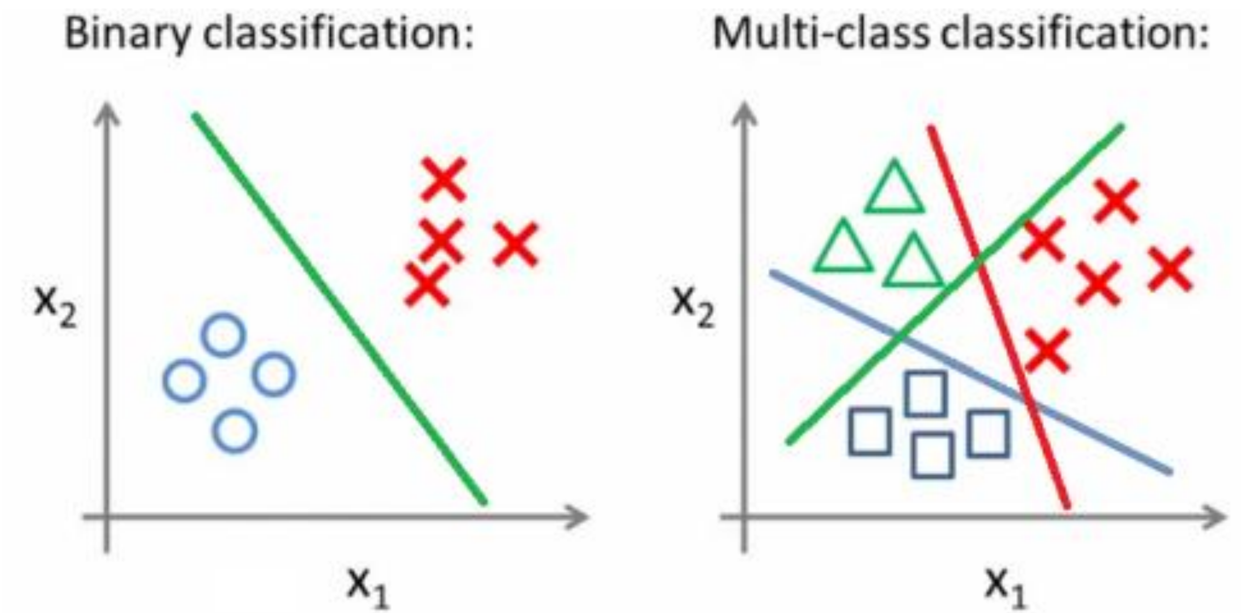



Picture from: James Hays – Machine Learning Overview

# Binary vs Multi-class Classification



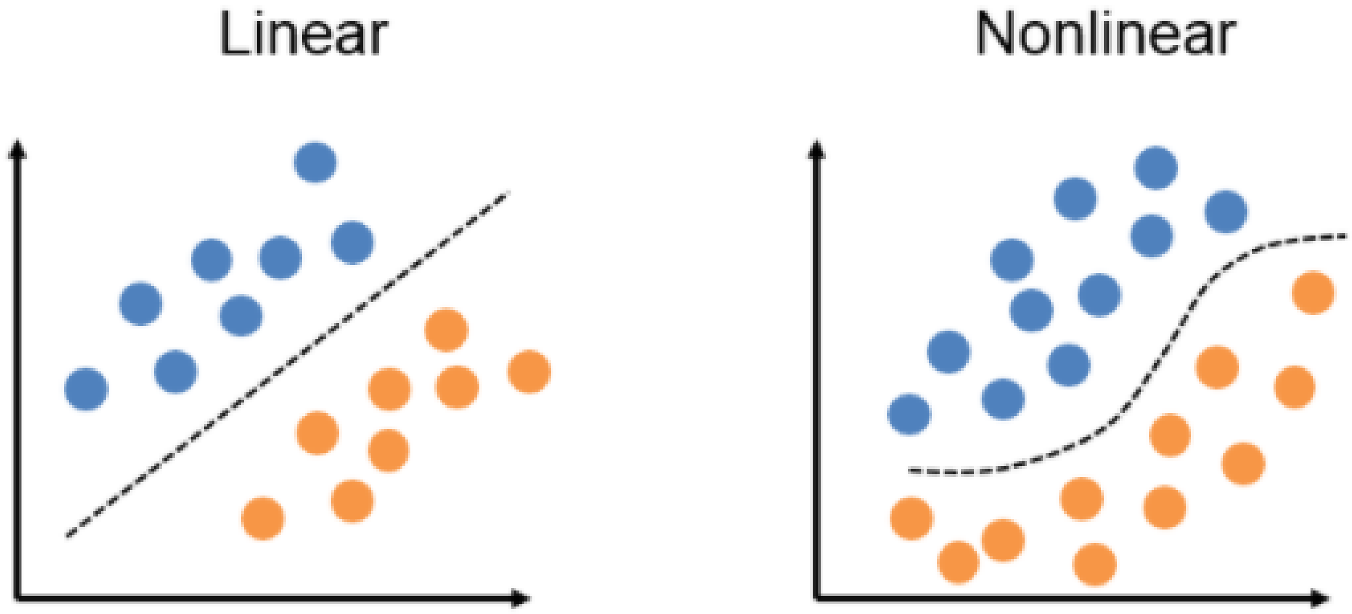
- A classification problem with only 2 classes is referred to as ***binary classification***
  - The output labels are 0 or 1
  - E.g., benign or malignant tumor, spam or no-spam email
- A problem with 3 or more classes is referred to as ***multi-class classification***



# Binary vs Multi-class Classification



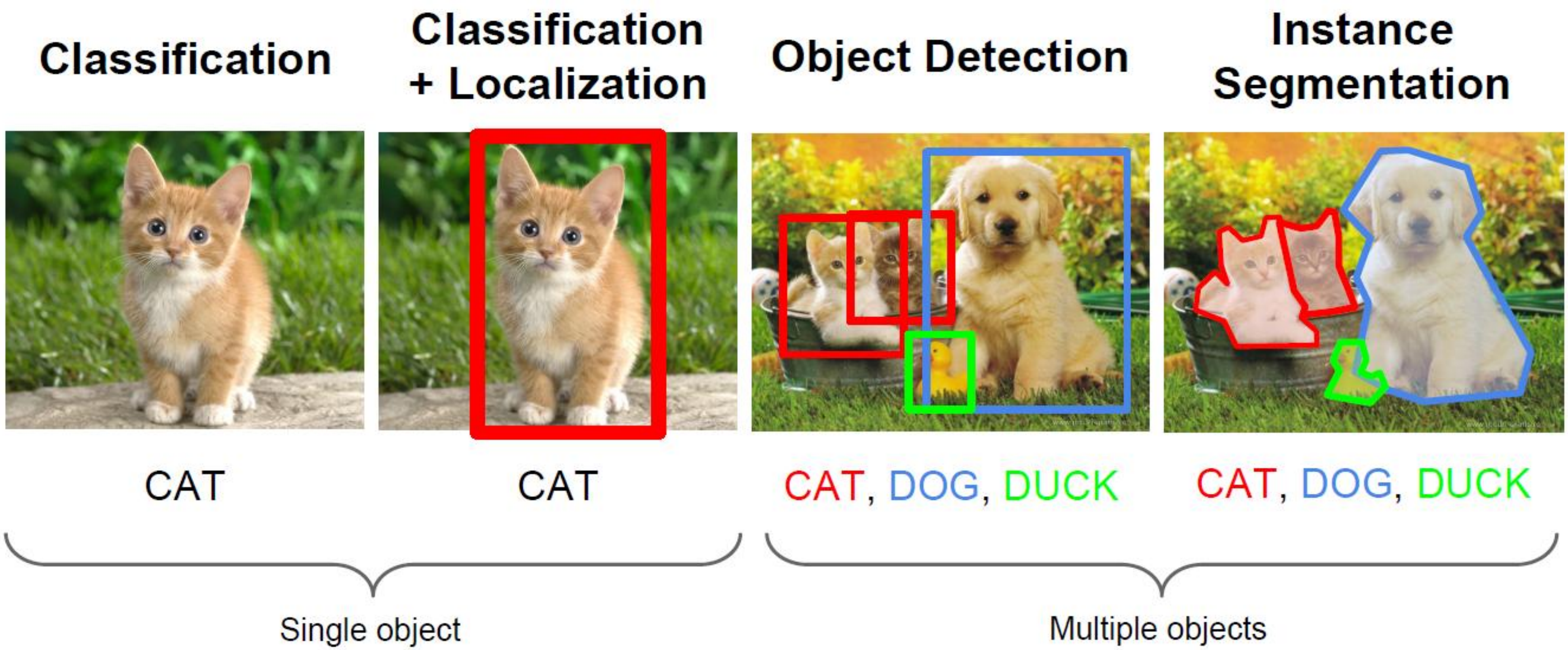
- Both the binary and multi-class classification problems can be linearly or non-linearly separated
  - Figure: linearly and non-linearly separated data for binary classification problem



# Computer Vision Tasks

*Machine Learning Basics*

- Computer vision has been the primary area of interest for ML
- The tasks include: classification, localization, object detection, instance segmentation




Picture from: Fie-Fei Li, Andrej Karpathy, Justin Johnson – Understanding and Visualizing CNNs

# No-Free-Lunch Theorem



- Wolpert (2002) - The Supervised Learning No-Free-Lunch Theorems
- The derived classification models for supervised learning are simplifications of the reality
  - The simplifications are based on certain assumptions
  - The assumptions fail in some situations
    - E.g., due to inability to perfectly estimate ML model parameters from limited data
- In summary, ***No-Free-Lunch Theorem*** states:
  - **No single classifier works the best for all possible problems**
  - Since we need to make assumptions to generalize