Learning by Computing Distances: Distance-based Methods and Nearest Neighbors

Piyush Rai

Machine Learning (CS771A)

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Data and Data Representation

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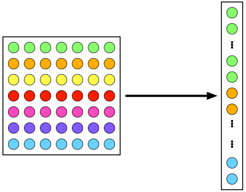

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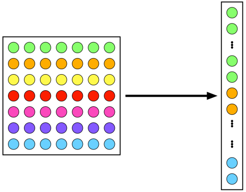

  - Note: Good features can also be learned from data (feature learning) or extracted using hand-crafted rules defined by a domain expert
- Output y_n can be real-valued, categorical, or a structured object, depending on the problem (regression, classification, structured output learning, etc.)

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$$d(\boldsymbol{x}_n, \boldsymbol{x}_m) = ||\boldsymbol{x}_n - \boldsymbol{x}_m|| = \sqrt{(\boldsymbol{x}_n - \boldsymbol{x}_m)^\top (\boldsymbol{x}_n - \boldsymbol{x}_m)} = \sqrt{\sum_{d=1}^{D} (x_{nd} - x_{md})^2}$$

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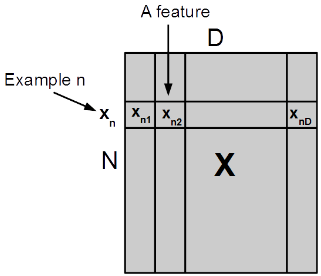
  - ℓ_1 distance between two points $\boldsymbol{x}_n$ and $\boldsymbol{x}_m$

$$d_1(\boldsymbol{x}_n, \boldsymbol{x}_m) = ||\boldsymbol{x}_n - \boldsymbol{x}_m||_1 = \sum_{d=1}^{D} |x_{nd} - x_{md}|$$

More on Data Representation..

We will (usually) assume that:

- $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ denotes data in form of an $N \times D$ feature matrix
- N examples, D features to represent each example
- Each row is an example, each column is a feature
- $\boldsymbol{x}_n$ denotes the n-th example (a vector of length D)



Data Matrix
(Rows: examples, columns: features)

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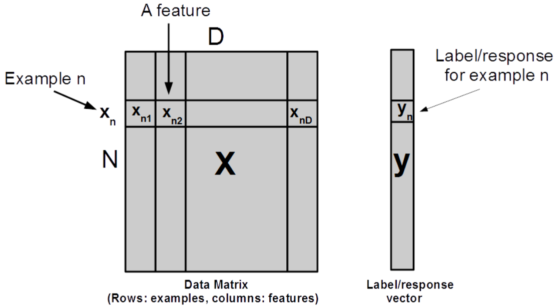
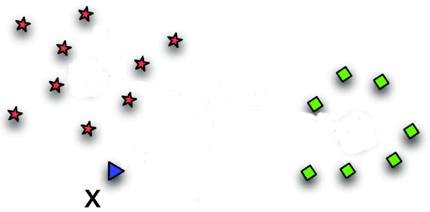


- $\boldsymbol{y}$ denotes labels/responses in form of an $N \times 1$ label/response vector
- y_n denotes label/response of the n-th example $\boldsymbol{x}_n$

Our First Learning Algorithm

A Simple Distance-based Classifier

- Given: N labeled training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$ from two classes
    - Assume green is positive and red is negative class
    - N_+ exampes from positive class, N_- examples from negative class
- Our goal: Learn a model to predict label (class) y for a new test example $\boldsymbol{x}$



Pic credit: Modified from the original by Alex Smola and Vishy Vishwanathan

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- A simple "distance from means" model: assign to class with closer mean
- Note: The basic idea generalizes to more than 2 classes as well

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- Note: We can simply store the two means and throw away the training data

Distance from Means: More Formally

- Distances from each mean are given by

$$||\boldsymbol{\mu}_- - \boldsymbol{x}||^2 = ||\boldsymbol{\mu}_-||^2 + ||\boldsymbol{x}||^2 - 2\langle \boldsymbol{\mu}_-, \boldsymbol{x}\rangle$$
$$||\boldsymbol{\mu}_+ - \boldsymbol{x}||^2 = ||\boldsymbol{\mu}_+||^2 + ||\boldsymbol{x}||^2 - 2\langle \boldsymbol{\mu}_+, \boldsymbol{x}\rangle$$

- Note: $||\boldsymbol{a} - \boldsymbol{b}||^2$ denotes squared Euclidean distance b/w two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$
- Note: $\langle \boldsymbol{a}, \boldsymbol{b}\rangle$ denotes inner product of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$
- Note: $||\boldsymbol{a}||^2 = \langle \boldsymbol{a}, \boldsymbol{a}\rangle$ denotes the squared ℓ_2 norm of $\boldsymbol{a}$

Distance from Means: The Decision Rule

- Let us denote by $f(\boldsymbol{x})$ our decision rule, defined as

$$f(\boldsymbol{x}) := ||\boldsymbol{\mu}_- - \boldsymbol{x}||^2 - ||\boldsymbol{\mu}_+ - \boldsymbol{x}||^2 = 2\langle \boldsymbol{\mu}_+ - \boldsymbol{\mu}_-, \boldsymbol{x}\rangle + ||\boldsymbol{\mu}_-||^2 - ||\boldsymbol{\mu}_+||^2$$

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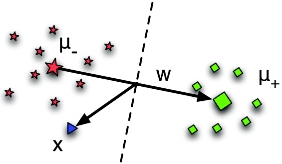

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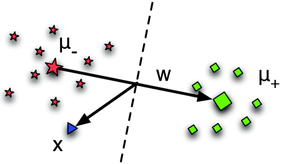

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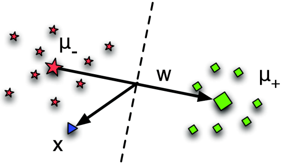

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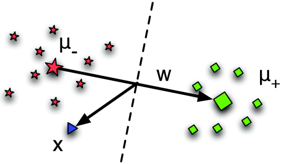

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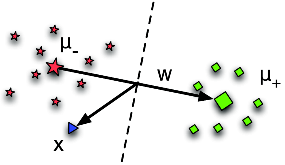
  - The inner product above can be replaced by more general similarity functions

Some aspects of "Distance from Means"



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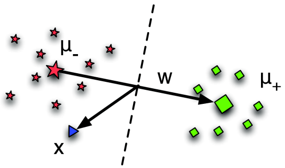

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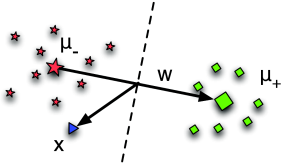

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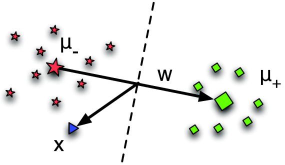

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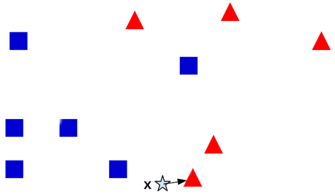
- Can be made more rigorous by modeling each class by a more sophisticated class probability distribution (e.g., a multivariate Gaussian) and computing distances of test points from these class distributions (rathar than means)
  - Several methods have this flavor, e.g., Linear (Fisher) Discriminant Analysis

Nearest Neighbor Methods

Nearest Neighbor

- Another classic distance-based supervised learning method



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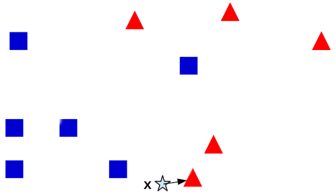

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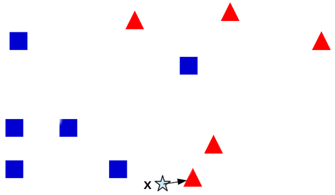

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- Note: The method also applies to regression problems (real-valued labels)

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Some Aspects about Nearest Neighbor

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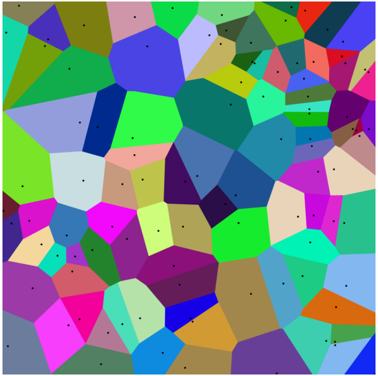
- The 1-NN can suffer if data contains outliers (we will soon see a geometric illustration), or if amount of training data is small. Using more neighbors ($K > 1$) is usually more robust

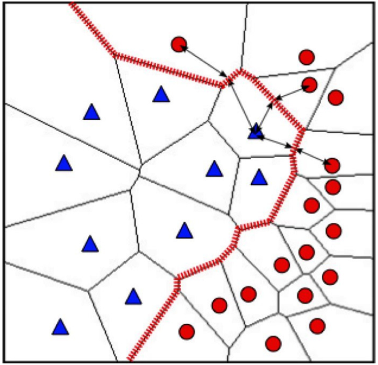
Geometry of 1-NN

- 1-NN induces a Voronoi tessellation of the input space



The Decision Boundary of 1-NN

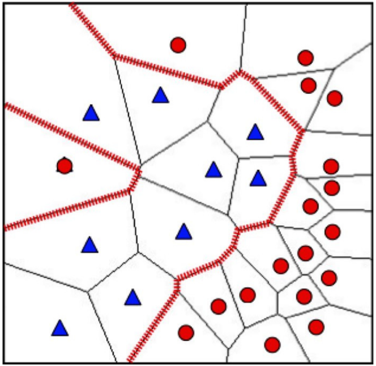
- The decision boundary is composed of hyperplanes that form perpendicular bisectors of pairs of points from different classes



Pic credit: Victor Lavrenko

Effect of Outliers on 1-NN

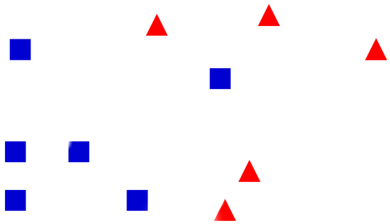
- An illustration of how the decision boundary can drastically change when the data contains some outliers



Pic credit: Victor Lavrenko

K-Nearest Neighbors (K-NN)

- Makes one-nearest-neighbor more robust by using more than one neighbor
- The K-NN prediction rule: Take a majority vote (or average) of the labels of $K > 1$ neighbors in the training data



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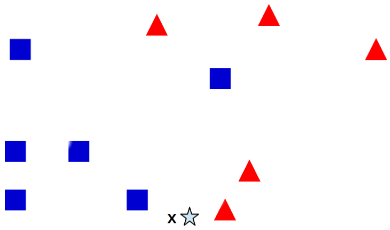

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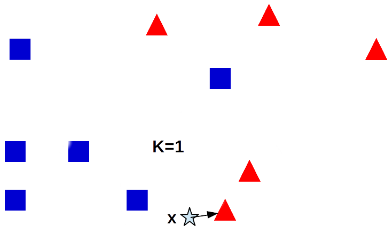

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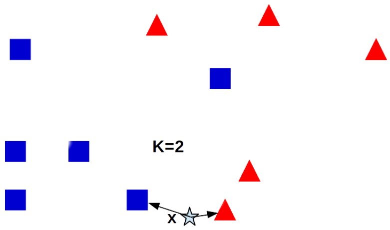

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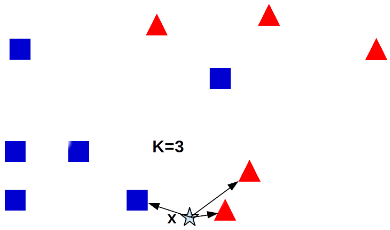

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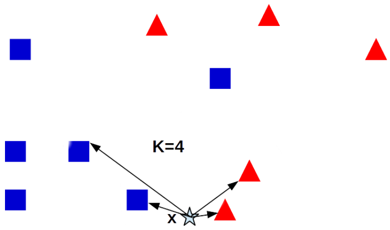

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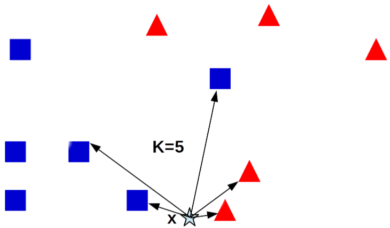

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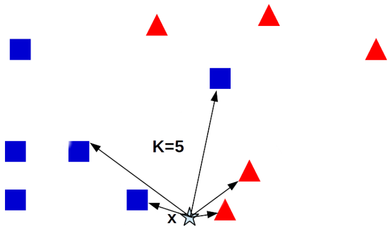

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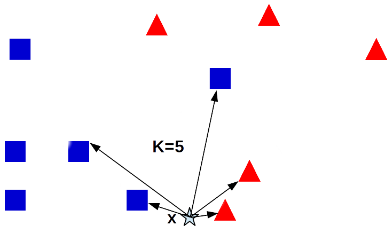

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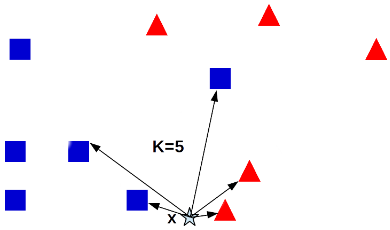

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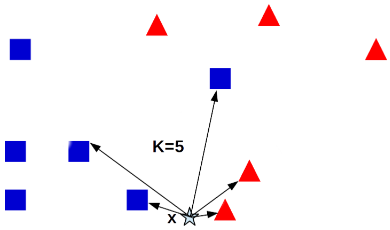

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  - For classification, we usually take the majority labels from the K neighbors
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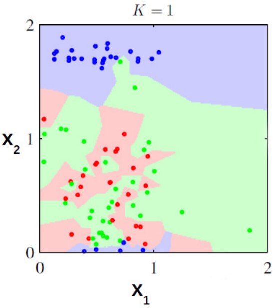
- The "right" value of K needs to be selected (e.g., via cross-validation)

- Larger K leads to smoother decision boundaries



Pic credit: Chris Bishop (PRML)

K-Nearest Neighbors: Decision Boundaries

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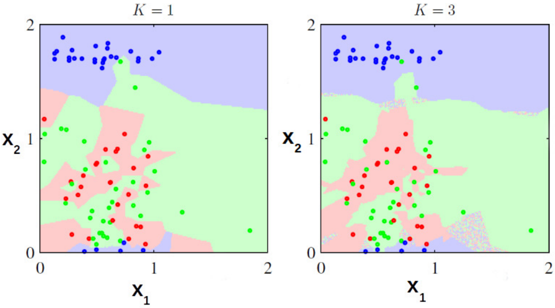

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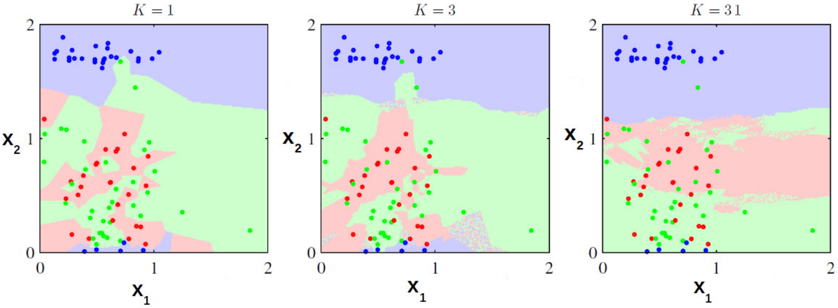

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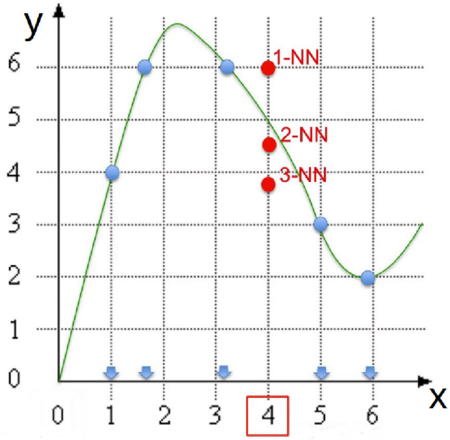
K-NN Behavior for Regression



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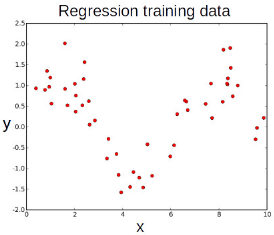

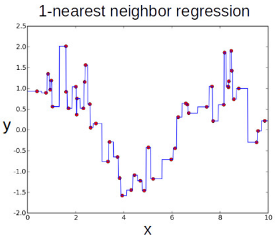

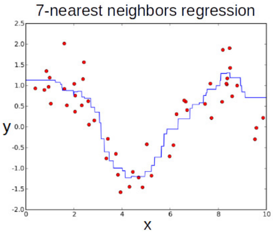

Pic credit: Alex Smola and Vishy Vishwanathan

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  - A "Distance from Means" Method
  - Nearest Neighbors Method
- Both are simple to understand and only require knowledge of basic geometry
- Have connections to other more advanced methods (as we will see)
- Need to be careful when computing the distances (or when deciding which distance function to use). Euclidean distance may not work well in many cases, especially in high dimensions (or may have to do some careful scaling of features if different features are not on the same scale)

Next Class:
Decision Trees for Classification and Regression