Warming-up to ML, and Some Simple Supervised Learners (Distance-based "Local" Methods)

Piyush Rai

Introduction to Machine Learning (CS771A)

August 2, 2018

Announcements

- Please sign-up on Piazza if you haven't already

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- I'll be clearing all the add-drop requests by tomorrow
- Maths refresher tutorial on Aug 4, 6:00-7:30pm in RM-101
  - Will be mostly on the basics of multivariate calculus, linear algebra, prob/stats, optimization (basically things you are expected to know for this course)

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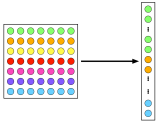

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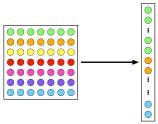

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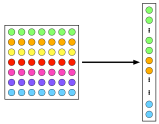

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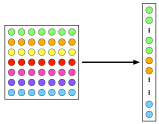

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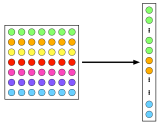

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  - The output y_n can be a scalar, a vector of numbers, or a structured object (more on this later)

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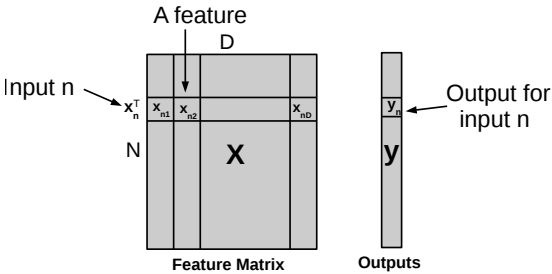

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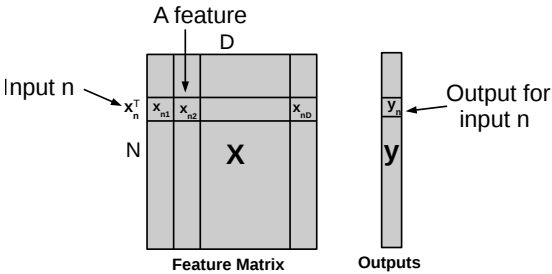

- Note: If each y_n itself is a vector (we will see such cases later) then we will use a matrix $\mathbf{Y}$ to collectively denote all the N outputs (with row n containing y_n) and also use boldfaced $\boldsymbol{y}_n$

Getting Features from Raw Data: A Simple Example

Consider the feature representation for some text data consisting of the following sentences:

- John likes to watch movies
- Mary likes movies too
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Again, note that this may not necessarily be the best "feature" representation for a given task (which is why other techniques or feature learning may be needed)

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- In Sup. Learning, different types of outputs may require different type of learning models

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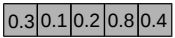

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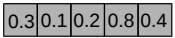

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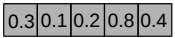

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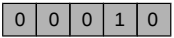

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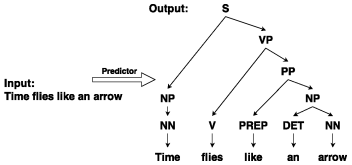
- Note: Multi-label classification is also informally called "tagging" (especially in Computer Vision)

Supervised Learning (Contd.)

- Structured-Prediction (a.k.a. Structured Output Learning): Each y_n is a structured object



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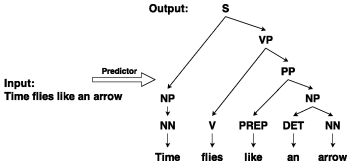

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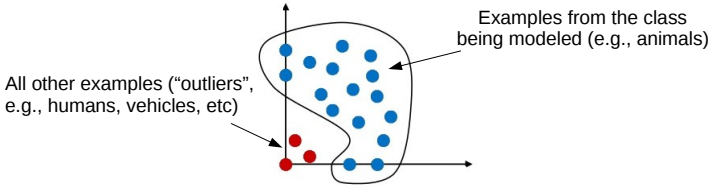

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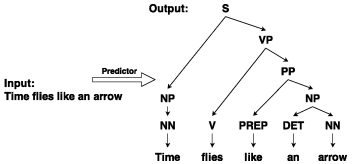

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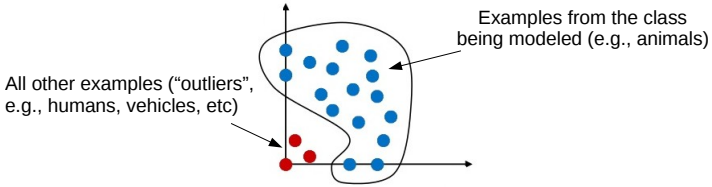

- Ranking: Each y_n is a ranked list of relevant stuff for a given input/query $\boldsymbol{x}$

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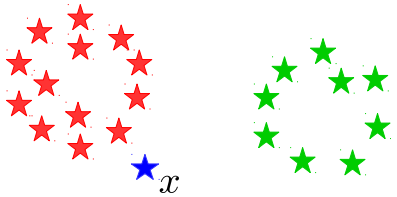
$$d_1(\boldsymbol{x}_n, \boldsymbol{x}_m) = ||\boldsymbol{x}_n - \boldsymbol{x}_m||_1 = \sum_{d=1}^{D} |x_{nd} - x_{md}|$$

Our First (Supervised) Learning Algorithm

Our First (Supervised) Learning Algorithm (need to know nothing except how to compute distances/similarities between points!)

Prototype based Classification

- 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 $\boldsymbol{x}$



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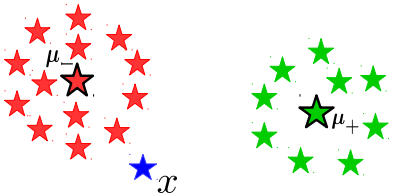

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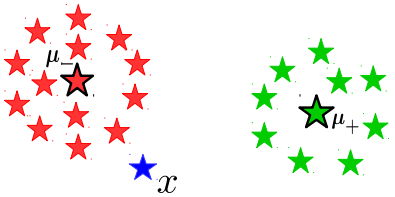
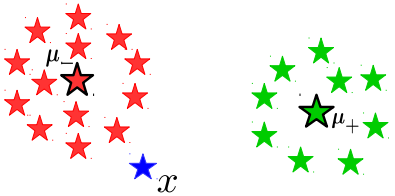


- A simple "distance from means" model: predict the class that has a closer mean
- Note: The basic idea easily generalizes to more than 2 classes as well

Prototype based Classification: More Formally

- What does the decision rule look like, mathematically ?



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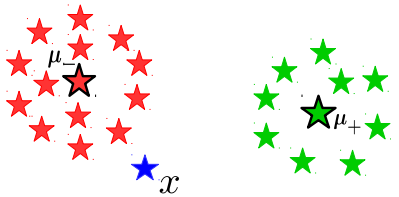

- The mean of each class is given by

$$\boldsymbol{\mu}_- = \frac{1}{N_-} \sum_{y_n=-1} \boldsymbol{x}_n \quad \text{and} \quad \boldsymbol{\mu}_+ = \frac{1}{N_+} \sum_{y_n=+1} \boldsymbol{x}_n$$

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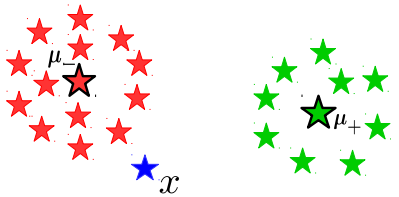

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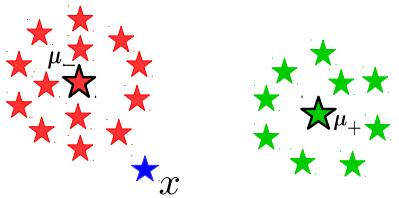

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- **Decision Rule:** If $f(\boldsymbol{x}) := ||\boldsymbol{\mu}_- - \boldsymbol{x}||^2 - ||\boldsymbol{\mu}_+ - \boldsymbol{x}||^2 > 0$ then predict +1, otherwise predict -1

Prototype based Classification: The Decision Rule

- We saw that our decision rule was

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

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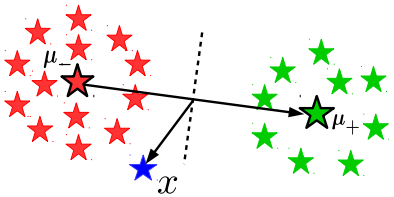
- **Imp.:** $f(\boldsymbol{x})$ effectively denotes a hyperplane based classification rule $f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b$ with the vector $\boldsymbol{w} = \boldsymbol{\mu}_+ - \boldsymbol{\mu}_-$ representing the direction normal to the hyperplane



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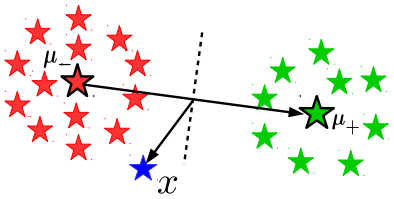

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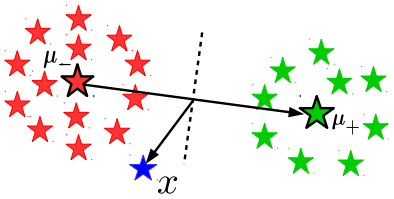

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  - This form of the decision rule is very important. Decision rules for many (in fact most) supervised learning algorithms can be written like this (weighted sum of similarities with all the training inputs)

Be Careful when Computing Distances

- Euclidean distance $d(\boldsymbol{x}_n, \boldsymbol{x}_m) = \sqrt{(\boldsymbol{x}_n - \boldsymbol{x}_m)^\top (\boldsymbol{x}_n - \boldsymbol{x}_m)}$ may not always be appropriate

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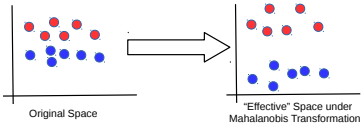

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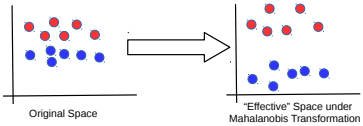

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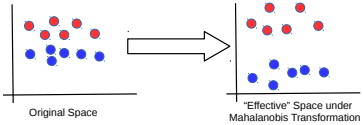

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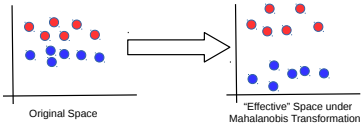

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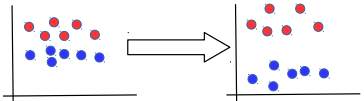

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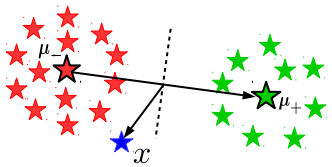

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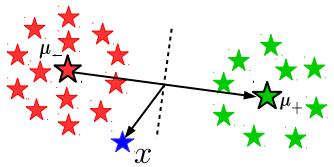

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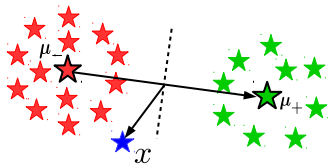

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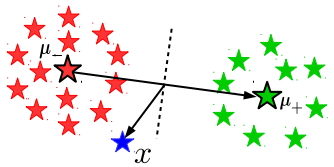

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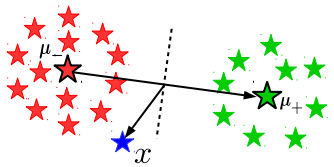

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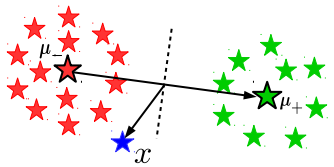

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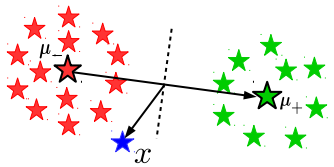

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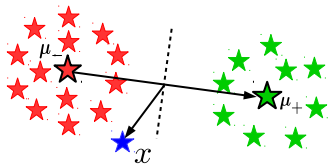

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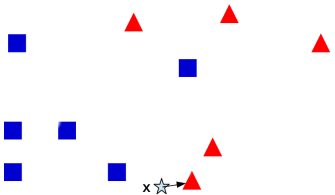
  - But with a good feature learner, even ONE (or very few) example per class may be enough (a state-of-the-art "Few-Shot Learning" model actually uses Prototype based classification)

Another Simple Supervised Learner: Nearest Neighbors

Nearest Neighbor

- Another classic distance-based supervised learning method



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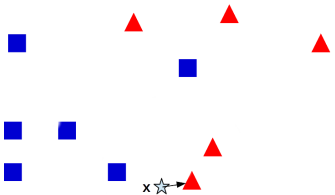

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- We typically use more ($K > 1$) neighbors in practice

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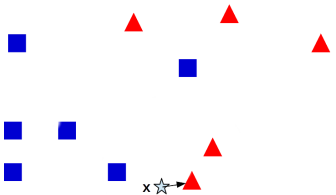
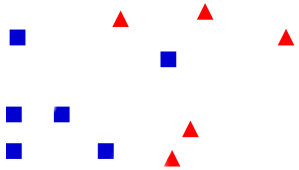
- Another classic distance-based supervised learning method



- The label y for $\boldsymbol{x} \in \mathbb{R}^D$ will be the label of its nearest neighbor in training data. Also known as one-nearest-neighbor (1-NN)
- Euclidean/Mahalanobis distance can be used to find the nearest neighbor (or can use a learned distance metric)
- We typically use more ($K > 1$) neighbors in practice
- Note: The method is widely applicable - works for both classification and regression problems

K-Nearest Neighbors (K-NN)

- Makes one-nearest-neighbor more robust by using more than one neighbor
- Test time simply does a majority vote (or average) of the labels of K closest training inputs



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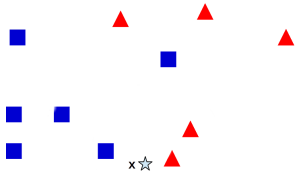

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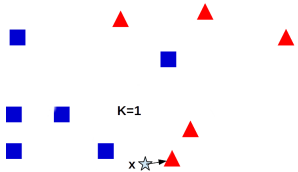

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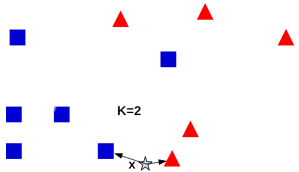

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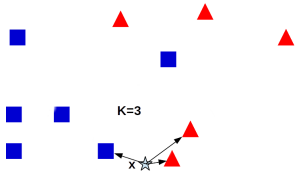

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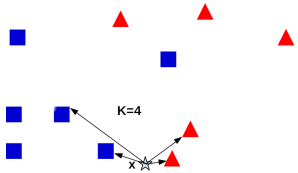

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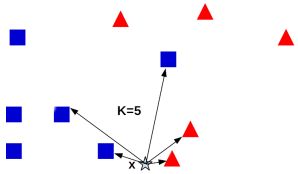

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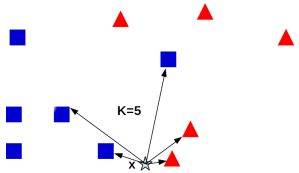

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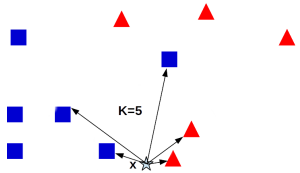

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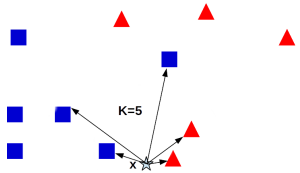

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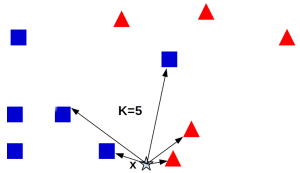

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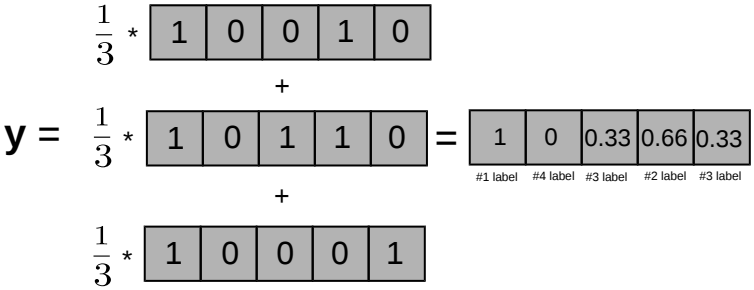
  - Averaging will give a real-valued "label score vector" $\boldsymbol{y} \in \mathbb{R}^M$ using which we can find the best label(s)

K-NN for Multi-Label Learning: Pictorial Illustration

- Suppose $K = 3$. The label averaging for a multi-label learning problem will look like



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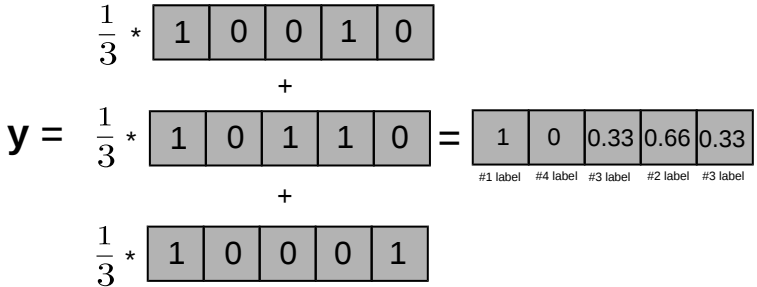

- Note that we can use the final $\boldsymbol{y}$ to rank the labels based on the real-valued scores
  - Can use it to predict the best, best-2, best-3, and so on..
  - Note: This is why multi-label learning is often used in some ranking problems where we wish to predict a ranking of the possible labels an input can have

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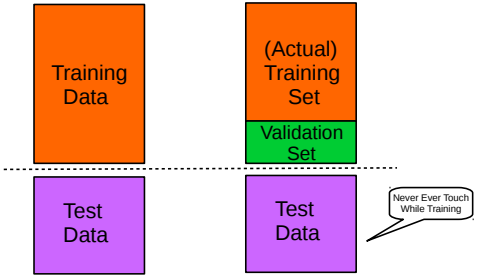

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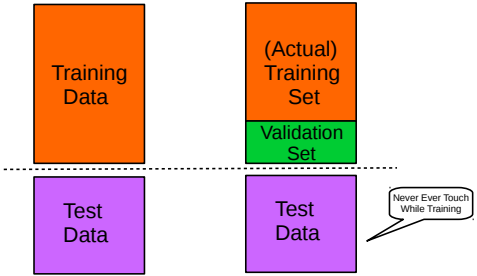

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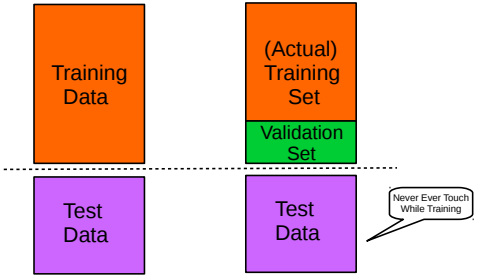

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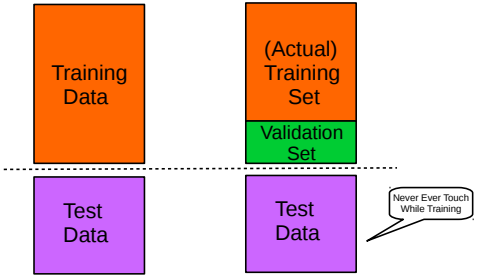

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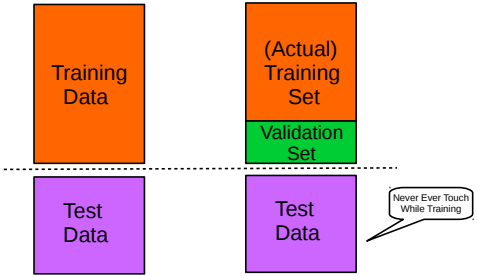
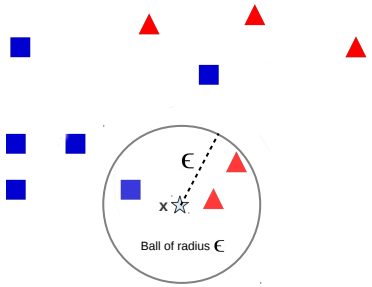


- Try different values of K and look at the accuracies on the validation set
  - Note: For each K, we typically try multiple splits of train and validation sets
- Select the K that gives the best accuracy on the validation set
- Never touch the test set (even if you have access to it) during training to choose the best K

ϵ-Ball Nearest Neighbors

- Instead of K nearest neighbors, can instead consider an ϵ-radius ball centered at the test point



- Just like selecting K, we can select the optimal ϵ via cross-validation
- Have to be careful to choose ϵ so as to not get zero neighbors within ϵ-ball :-)

Some Aspects about Nearest Neighbor

- A simple yet very effective method in practice (if given lots of training data)
  - *Provably* has an error-rate that is no worse than twice of the "Bayes optimal" classifier which assumes knowledge of the true data distribution for each class

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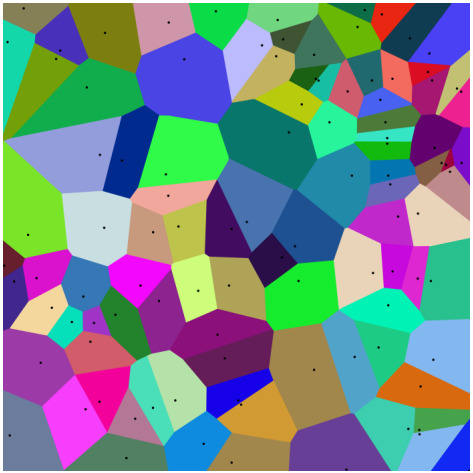
- Need to be careful in choosing the distance function to compute distances (especially when the data dimension D is very large)
- The 1-NN can suffer if data contains outliers (we will soon see a geometric illustration), or if amount of training data is small. Using more neighbors ($K > 1$) is usually more robust

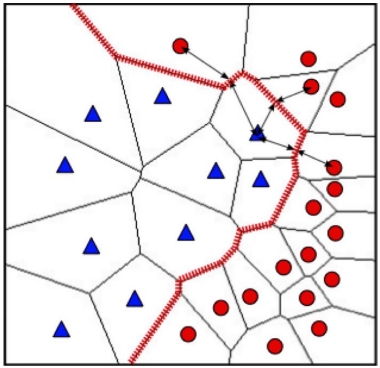
Geometry of 1-NN

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



The Decision Boundary of 1-NN (for binary classification)

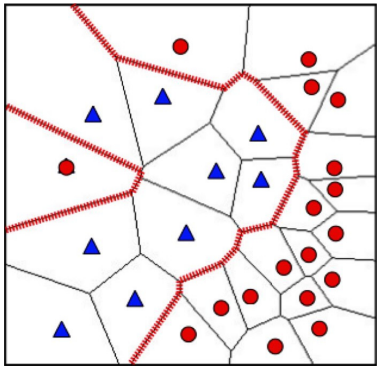
- The decision boundary is composed of hyperplanes that form perpendicular bisectors of pairs of points from different classes



Pic credit: Victor Lavrenko

Effect of Outliers on 1-NN

- How the decision boundary can drastically change when the data contains some outliers



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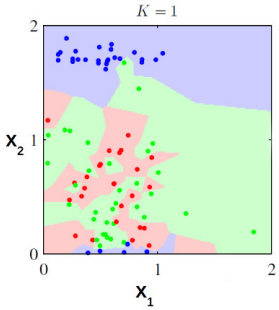
Effect of Varying K

- Larger K leads to smoother decision boundaries



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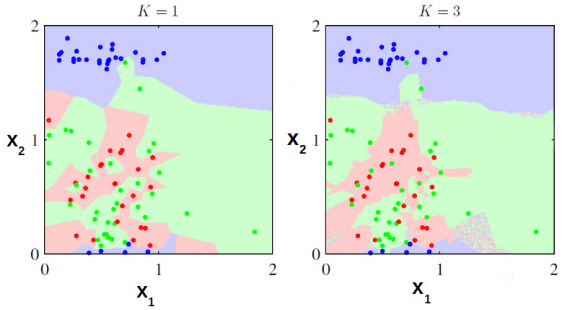

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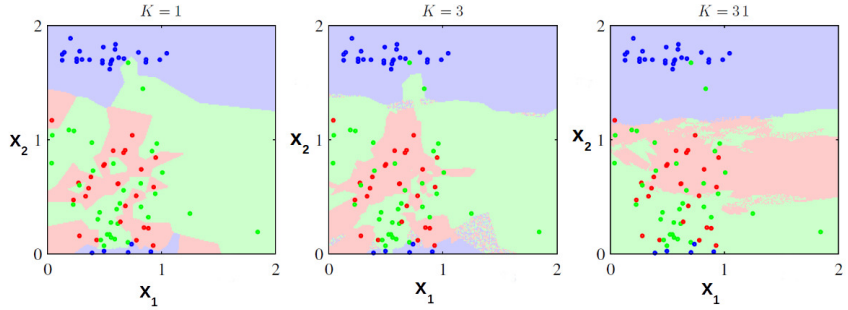

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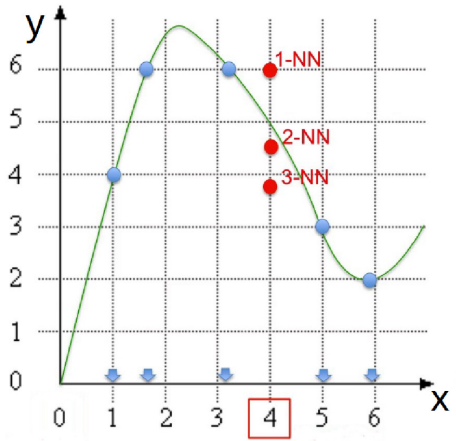
K-NN Behavior for Regression



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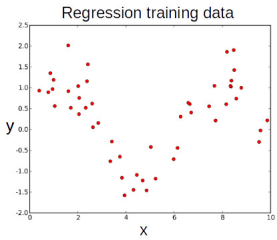

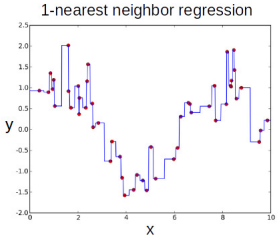

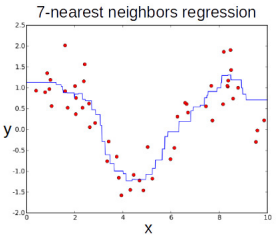

Pic credit: Alex Smola and Vishy Vishwanathan

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- Have connections to other more advanced methods (as we will see)
- Need to be careful when computing the distances (learned Mahalanobis distance metrics, or "learned features" + Euclidean distance can often do wonders!)