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

Piyush Rai

Introduction to Machine Learning (CS771A)

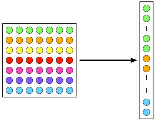
August 2, 2018

Announcements

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

Some Notation/Nomenclature/Convention

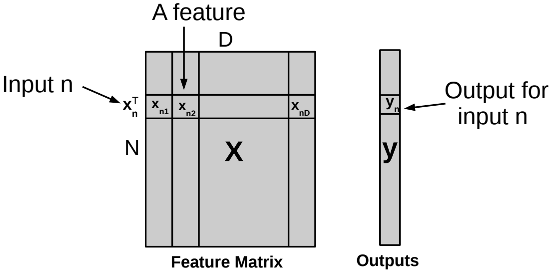
- Supervised Learning requires training data given as a set of input-output pairs $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$
- Unsupervised Learning requires training data given as a set of inputs $\{\boldsymbol{x}_n\}_{n=1}^N$
- Each input $\boldsymbol{x}_n$ is (usually) a vector containing the values of the features or attributes or covariates that encode properties of the data it represents, e.g.,
  - Representing a 7×7 image: $\boldsymbol{x}_n$ can be a 49×1 vector of pixel intensities



  - Note: Good features can also be learned from data (feature learning) or extracted using hand-crafted rules defined by a domain expert. **Having a good set of features is half the battle won!**
- Each y_n is the output or response or label associated with input $\boldsymbol{x}_n$
  - The output y_n can be a scalar, a vector of numbers, or a structured object (more on this later)

Some Notation/Nomenclature/Convention

- Will assume each input $\boldsymbol{x}_n$ to be a $D \times 1$ column vector (its transpose $\boldsymbol{x}_n^\top$ will be row vector)
- x_{nd} will denote the d-th feature of the n-th input
- We will use $\mathbf{X}$ ($N \times D$ feature matrix) to collectively denote all the N inputs
- We will use $\boldsymbol{y}$ ($N \times 1$ output/response/label vector) to collectively denote all the N outputs



- 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
- John also likes football

Our feature "vocabulary" consists of 8 unique words

Here is the **bag-of-words** feature vector representation of these 3 sentences

$$\begin{array}{c} \\ \text{Sentence 1} \\ \text{Sentence 2} \\ \text{Sentence 3} \end{array} \begin{pmatrix} \text{John} & \text{likes} & \text{to} & \text{watch} & \text{movies} & \text{Mary} & \text{too} & \text{also} & \text{football} \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

Here the features are binary (presence/absence of each word)

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)

Types of Features and Types of Outputs

- Features (in vector $\boldsymbol{x}_n$) as well as outputs y_n can be real-valued, binary, categorical, ordinal, etc.
- Real-valued: Pixel intensity, house area, house price, rainfall amount, temperature, etc
- Binary: Male/female, adult/non-adult, or any yes/no or present/absent type values
- Categorical/Discrete: Pincode, bloodgroup, or any "which one from this finite set" type values
- Ordinal: Grade (A/B/C etc.) in a course, or any other type where relative values matters
- Often, the features can be of mixed types (some real, some categorical, some ordinal, etc.)
- Appropriate handling of different types of features may be very important (even if you algorithm is designed to "learn" good features, given a set of heterogeneous features)
- In Sup. Learning, different types of outputs may require different type of learning models

Supervised Learning

Supervised Learning

- Supervised Learning comes in many flavors. The flavor depends on the type of each output y_n
- Regression: $y_n \in \mathbb{R}$ (real-valued scalar)
- Multi-Output Regression: $\boldsymbol{y}_n \in \mathbb{R}^M$ (real-valued vector containing M outputs)

0.3	0.1	0.2	0.8	0.4

Illustration of a 5-dim output vector for a multi-output regression problem

- Binary Classification: $y_n \in \{-1, +1\}$ or $\{0, 1\}$ (output in classification is also called "label")
- Multi-class Classification: $y_n \in \{1, 2, \ldots, M\}$ or $\{0, 1, \ldots, M-1\}$ (one of M classes is correct label)

0	0	0	1	0

Illustration of a 5-dim one-hot label vector for a multi-class classification problem

- Multi-label Classification: $y_n \in \{-1, +1\}^M$ or $\{0, 1\}^M$ (a subset of M labels are correct)

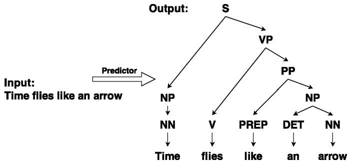
1	0	1	0	0

Illustration of a 5-dim binary label vector for a multi-label classification problem (unlike one-hot, there can be multiple 1s)

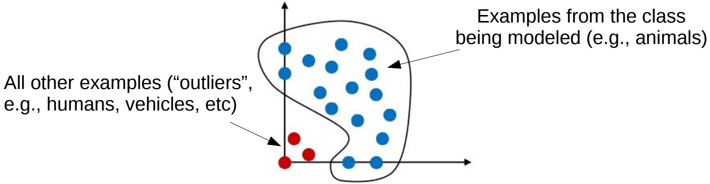
- Note: Multi-label classification is also informally called "tagging" (especially in Computer Vision)

Supervised Learning (Contd.)

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



- One-Class Classification (a.k.a. outlier/anomaly/novelty detection): y_n is "1" or "everything else"



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

Background: Computing Distances/Similarities

- Assuming all real-valued features, an input $\boldsymbol{x}_n \in \mathbb{R}^{D \times 1}$ is a point in a D dim. vector space of reals
- Standard rules of vector algebra apply on such representations, e.g.,
  - Euclidean distance b/w two points (say two images or two documents) $\boldsymbol{x}_n \in \mathbb{R}^D$ and $\boldsymbol{x}_m \in \mathbb{R}^D$

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

  - Inner-product similarity b/w $\boldsymbol{x}_n$ and $\boldsymbol{x}_m$ (cosine, $\boldsymbol{x}_n$, $\boldsymbol{x}_m$ are unit-length vectors)

$$s(\boldsymbol{x}_n, \boldsymbol{x}_m) = \langle \boldsymbol{x}_n, \boldsymbol{x}_m \rangle = \boldsymbol{x}_n^\top \boldsymbol{x}_m = \sum_{d=1}^{D} x_{nd} x_{md}$$

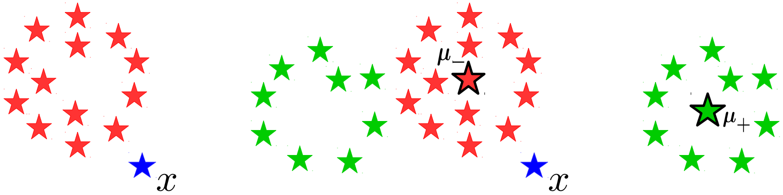
  - ℓ_1 distance between two points $\boldsymbol{x}_n$ and $\boldsymbol{x}_m$

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

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

Prototype based Classification

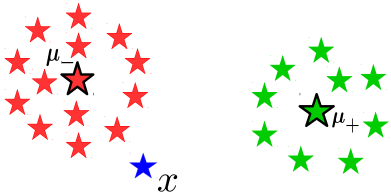
- Given: N labeled training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$ from two classes
  - Assume green is positive and red is negative class
  - N_+ exampes from positive class, N_- examples from negative class
- Our goal: Learn a model to predict label (class) y for a new test example $\boldsymbol{x}$



- 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 ?



- The mean of each class is given by

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

- Euclidean Distances from each mean are given by

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

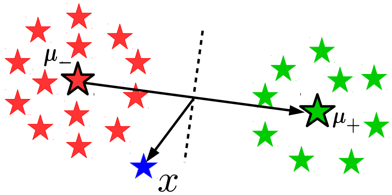
- **Decision Rule:** If $f(\boldsymbol{x}) := ||\boldsymbol{\mu}_- - \boldsymbol{x}||^2 - ||\boldsymbol{\mu}_+ - \boldsymbol{x}||^2 > 0$ then predict $+1$, otherwise predict -1

Prototype based Classification: The Decision Rule

- We saw that our decision rule was

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

- **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



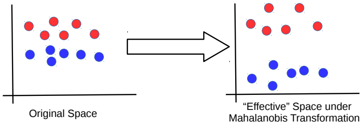
- **Imp.:** Can show that the rule is equivalent to $f(\boldsymbol{x}) = \sum_{n=1}^N \alpha_n \langle \boldsymbol{x}_n, \boldsymbol{x}\rangle + b$, where α's and b can be estimated from training data **(try this as an exercise)**
  - This form of the decision rule is very important. Decision rules for 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
- Another alternative (still Euclidean-like) can be to use the Mahalanobis distance

$$d_M(\boldsymbol{x}_n, \boldsymbol{x}_m) = \sqrt{(\boldsymbol{x}_n - \boldsymbol{x}_m)^\top \mathbf{M} (\boldsymbol{x}_n - \boldsymbol{x}_m)}$$

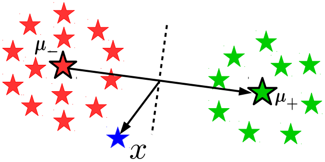
- Shown below is an illustration of what $\mathbf{M} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$ will do (note: figure not to scale)



- How do I know what's the right **M** for my data?Some options
  - Set it based on some knowledge of what you data looks like
  - Learn it from data (called Distance Metric Learning[1] - a whole reseach area in itself)
- Distance Metric Learning is one of the many approaches for feature learning from data

[1] Distance Metric Learning. See "A Survey on Metric Learning for Feature Vectors and Structured Data" by Ballet *et al*

Prototype based Classification: Some Comments

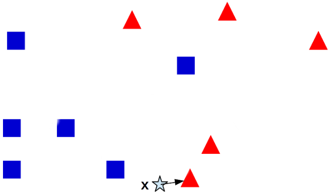


- A very simple supervised learner. Works for any number of classes. Trivial to implement. :-)
- This simple approach, if using Euclidean distances, can only learn linear decision boundaries
  - A reason: The basic approach implicitly assumes that classes are roughly spherical and equi-sized
- Several nice improvements/generalizations possible (some of which we will see in coming lectures)
  - Instead of a point (mean), model classes by prob. distributions (to account for class shapes/sizes)
  - Instead of Euclidean distances, can use non-Euclidean distances, distance metric learning, or "kernels"
- Another limitation: Needs plenty of training data from each class to reliably estimate the means
  - 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

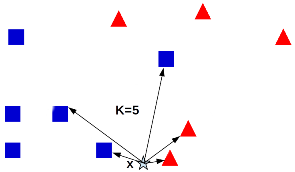
- Another classic distance-based supervised learning method



- 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



- For a test input $\boldsymbol{x}$, the averaging version of the prediction rule for K-nearest neighbors

$$\boldsymbol{y} = \frac{1}{K} \sum_{n \in \mathcal{N}_K(\boldsymbol{x})} \boldsymbol{y}_n$$

.. where $\mathcal{N}_K(\boldsymbol{x})$ is the set of K closest training inputs for $\boldsymbol{x}$

- Above assumes the K neighbors have equal $(1/K)$ weights. Can also use distance-based weights
- Note: The rule works for multi-label classification too where each $\boldsymbol{y}_n \in \{0,1\}^M$ is a binary vector
  - 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

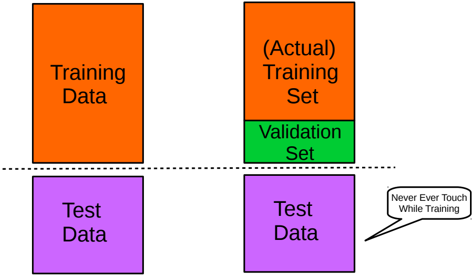
- Suppose $K = 3$. The label averaging for a multi-label learning problem will look like

$$\mathbf{y} = \frac{1}{3} * \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \end{bmatrix} + \frac{1}{3} * \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \end{bmatrix} + \frac{1}{3} * \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \end{bmatrix} = \begin{array}{ccccc} \begin{bmatrix} 1 & 0 & 0.33 & 0.66 & 0.33 \end{bmatrix} \\ \text{\#1 label} \quad \text{\#4 label} \quad \text{\#3 label} \quad \text{\#2 label} \quad \text{\#3 label} \end{array}$$

- 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

How to Select K: Cross-Validation

- We can use cross-validation to select the "optimal" value of K
- Cross-validation - Divide the training data into two parts: actual training set and a validation set



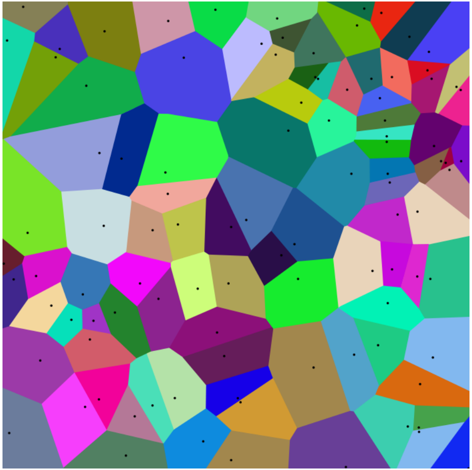
- Try different values of K and look at the accuracies on the validation set
  - Note: For each K, we typically try multiple splits of train and validation sets
- Select the K that gives the best accuracy on the validation set
- Never touch the test set (even if you have access to it) during training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

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
- Also called a memory-based or instance-based or non-parametric method
- No "model" is learned here. Prediction step uses all the training data
- Requires lots of storage (need to keep all the training data at test time)
- Predction can be slow at test time
  - For each test point, need to compute its distance from all the training points
  - Clever data-structures or data-summarization techniques can provide speed-ups
- 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

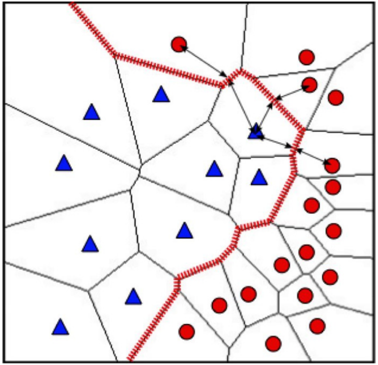
Geometry of 1-NN

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



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

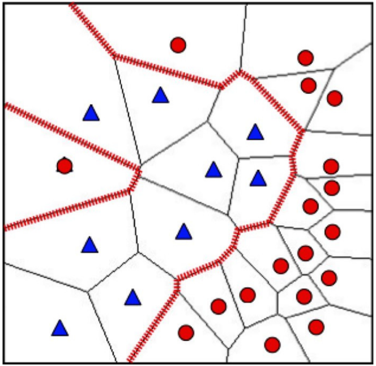
- The decision boundary is composed of hyperplanes that form perpendicular bisectors of pairs of points from different classes



Pic credit: Victor Lavrenko

Effect of Outliers on 1-NN

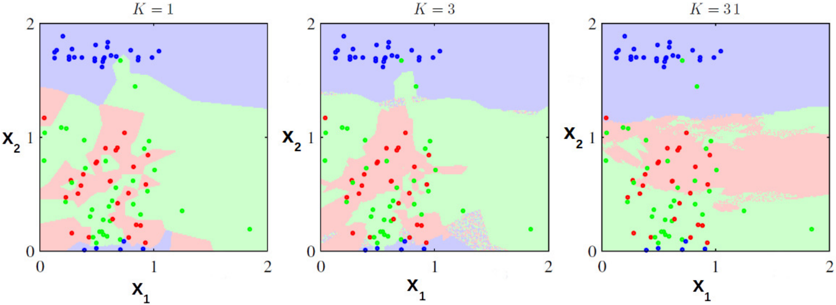
- How the decision boundary can drastically change when the data contains some outliers



Pic credit: Victor Lavrenko

Effect of Varying K

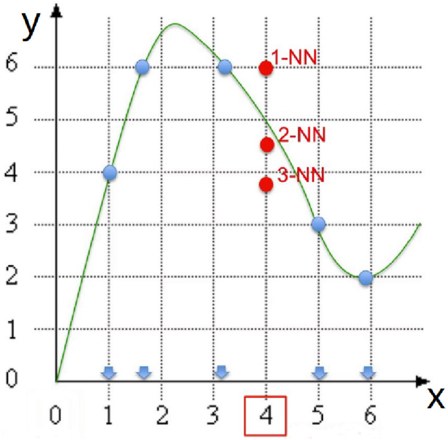
- Larger K leads to smoother decision boundaries



Too small K (e.g., $K = 1$) can lead to overfitting, too large K can lead to underfitting

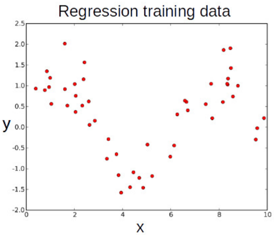
Pic credit: Chris Bishop (PRML)

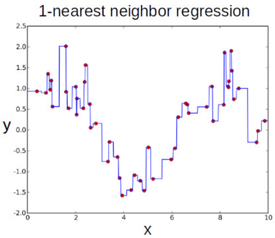
K-NN Behavior for Regression

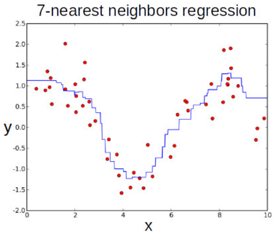


Pic credit: Victor Lavrenko

K-NN Behavior for Regression







Pic credit: Alex Smola and Vishy Vishwanathan

Summary

- Looked at two distance-based methods for classification/regression
  - A "Distance from Means" Method
  - Nearest Neighbors Method
- Both are essentially "local" methods (look at local neighborhood of the test point)
- 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 (learned Mahalanobis distance metrics, or "learned features" + Euclidean distance can often do wonders!)