STAT 534

Lecture 6

Kernel Density Estimation, Regression and Classification

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1 Introduction

In this lecture, we will discuss Nearest-Neighbor predictors and Kernel Density Estimation approaches on classification and regression problems.

1.1 Classification and Regression Problem

The classification and regression problems fall in a general category of machine learning tasks, the so-called supervised learning. Given a random pair $(X, Y) \in \mathcal{X} \times \mathcal{Y}$, the basic goal in supervised learning is to construct a prediction function f such that $Y = f(X)$ based on some training data. We often call X the *input*, *predictor*, *feature*, *independent variable*, etc., and Y the *output*, *response*, *dependent variable*, etc. Typically, the input space of X, i.e., $\mathcal{X}$, would simply be $\mathbb{R}^d$ and the training data comprises some (i.i.d.) samples from (X, Y), $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \mathcal{Y}, i = 1, ..., N\}$.
The difference between classification and regression problems emerges on the type of output variables.

- **Classification**: The output Y is *qualitative* and assumes values in a finite set. For instance, $\mathcal{Y} = \{-1, 1\}$.
- **Regression**: The output Y is a *quantitative* measurement, i.e., $\mathcal{Y} \subset \mathbb{R}$.

In a nutshell, the distinction in output type has led to a naming convention for the prediction tasks: *regression* when we predict quantitative outputs, and *classification* when we predict qualitative outputs. These two tasks have a lot in common, and in particular both can be viewed as a task in function approximation.[1]

1.2 Memory-Based Learning

The main topics of today's lecture, nearest-neighbor predictors and kernel density estimation methods, can be classified as examples of *memory-based learning* (sometimes called *instance-based learning*) within the realm of machine learning. **Memory-based learning** is based on the assumption that in learning a cognitive task from experience people do not extract rules or other abstract representations from their experience, but reuse their memory of that experience directly.[2] In other words, it compares new data instances with those seen in the training data, which have been stored in memory. Since

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it constructs hypotheses directly from the training instances themselves, the hypothesis complexity can grow with the data[3]: in the worst case, a hypothesis is a list of n training items and the computational complexity of classifying a single new instance is $\mathcal{O}(n)$.

1.3 Nonparametric Model

On the other hand, both Nearest-Neighbor predictors and kernel density estimation approaches are some vivid examplifications of nonparametric models, whose structures are not specified a priori but learned from data. This means that these statistical models are infinite-dimensional, in the sense that the number and nature of the parameters are grown with the size of data.

2 Nearest-Neighbor Predictor

Given a training data $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \mathcal{Y}, i = 1, ..., N\}$, the main idea of Nearest-Neighbor predictor is to assign the label or value of a new instance x as follows:

1. Find the example x^i that is nearest to x under a certain distance metric, says Euclidean distance. Mathematically, $i = \underset{j \in \{1,...,N\}}{\arg\min} ||x - x^j||_2$
2. Assign x the label or value y^i.

In practice, one uses the K nearest neighbors of x (with $K = 3, 5$ or larger). Then

- **For Classification**: $f(x) =$ the most frequent label among K nearest neighbors (the so-called *Majority Vote*).
- **For Regression**: $f(x) = \frac{1}{K} \sum_{i \text{ neighbor of } x} y^i =$ mean of neighbors' values.

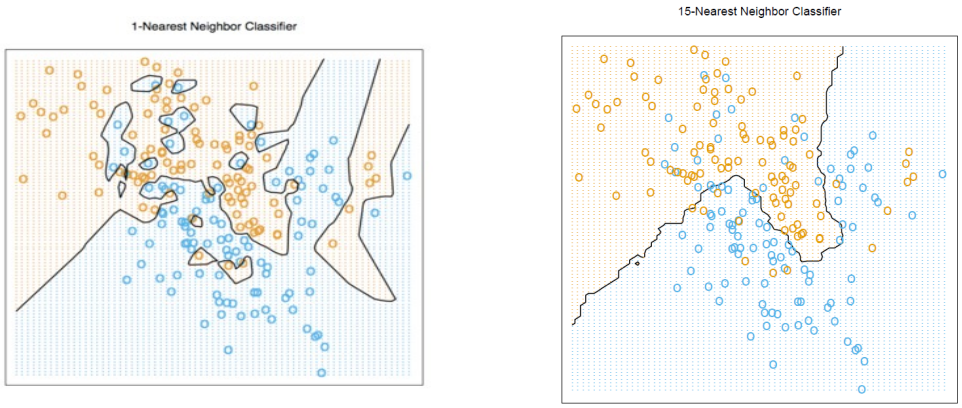
Figure 1 delineates an example when we apply the K-Nearest-Neighbor method on a binary classification problem, where those solid curves indicate the decision boundaries of two classifiers. In a binary classification problem, the **decision boundary** of a classifier is a hypersurface that partitions the underlying vector space into two sets, while the classifier will assign all the points on one side of the decision boundary to one class and all those on the other side to the other class. Upon the decision boundary, the output label of a classifier is ambiguous.[4] As shown by Figure 1, K serves as the smoothing parameter of the K-Nearest-Neighbor classifier, since the decision boundary becomes smoother as the value of K increases.

Remark. The decision boundary for a K-Nearest-Neighbor classifier is *piecewise linear*.

3 Kernel Density Estimation

Let $x^1, ..., x^N \in \mathbb{R}^d$ be an independent, identically distributed random sample from an unknown distribution P with density function p. Then the **Kernel Density Estimation** can be expressed as

$$\hat{p}_n(x) = \frac{1}{Nh^d} \sum_{i=1}^{N} b\left(\frac{x - x^i}{h}\right),$$



(a) 1-Nearest-Neighbor

(b) 15-Nearest-Neighbor

Figure 1: A Binary Classification Problem Using 1-Nearest-Neighbor and 15-Nearest-Neighbor Classifiers with Decision Boundaries[1]

where $b : \mathbb{R}^d \to \mathbb{R}$ is a smooth function such that $b(x) \geq 0$ and[5]

$$\int b(x)dx = 1, \int x \cdot b(x)dx = 0, \text{ and } \sigma_b^2 \equiv \int x^2 \cdot b(x)dx > 0,$$

and $h > 0$ is the bandwidth parameter that controls the amount of smoothing. b is called a kernel function. Two common examples of $b(x)$ are[6]

$$\text{(Gaussian kernel) } b(x) = \frac{\exp(-\frac{||x||^2}{2})}{v_{1,d}}, \; v_{1,d} = \int \exp\left(-\frac{||x||^2}{2}\right) dx,$$
$$\text{(Spherical Kernel) } b(x) = \frac{I(||x|| \leq 1)}{v_{2,d}}, \; v_{2,d} = \int I(||x|| \leq 1)dx.$$

Optional requirements on b are: (i) symmetric with respect to x and x^i, that is, $b(x, x^i) = b(x^i, x) = b\left(\frac{x-x^i}{h}\right)$; (ii) Radial symmetry; (iii) bounded support; (iv) higher order smoothness conditions, etc.

As with kernel regression, the choice of kernel b is not crucial, but the choice of bandwidth h is important.[5] Figure 2 shows density estimates with several different bandwidths using a part of the NACC (National Alzheimers Coordinating Center) Uniform Dataset, version 3.0 (March 2015).[6]

Roughly speaking, the computational cost of kernel density estimation is $\mathcal{O}(Nd)$, since we need to calculate the (Euclidean) distance of two d-dimensional data points. In Section 5 and subsequent lectures, we will introduce several efficient neighbor searching methods when the number of data points N is large.

[†] For instance, see https://stat.ethz.ch/R-manual/R-devel/library/stats/html/bandwidth.html for details

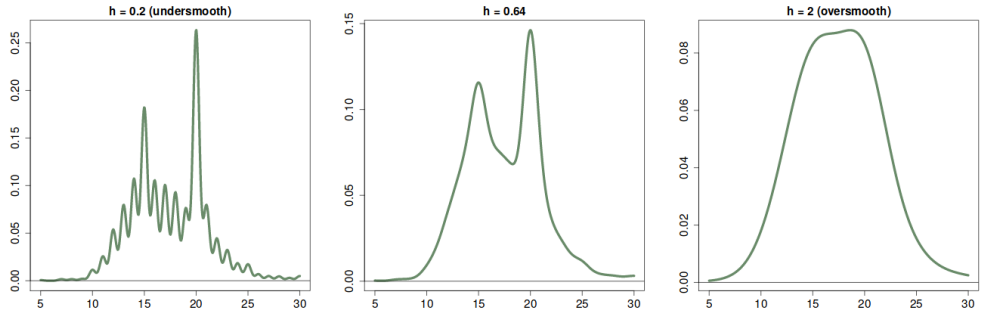


Figure 2: Kernel Density Estimation on Part of NACC Data. Left panel: undersmoothed. Middle panel: just right (bandwidth chosen by the default rule in R)[†]. Right panel: oversmoothed.

4 Kernel Regression and Classification

4.1 Kernel Regression

In any kernel regression setting, the conditional expectation of the response Y relative to the input X can be written as

$$f(X) = \mathbb{E}(Y|X).$$

As for a training data with i.i.d. samples $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \mathbb{R}, i = 1, ..., N\}$, we can always write

$$y^i = f(x^i) + \epsilon_i, \quad i = 1, ..., n,$$

where $\epsilon_i, i = 1, ..., n$ are i.i.d. random errors with mean zero. Like the K-Nearest-Neighbor approach, the kernel regression interpolates the value of a new data instance based on the neighbor values of this instance, but in a more "smoothed" way. Suppose that $b_h(x, x^i) = b\left(\frac{x-x^i}{h}\right)$, where b is a kernel function defined in Section 3. Then the **kernel regressor** can be written as

$$\hat{f}(x) = \sum_{i=1}^{N} \beta_i(x) \cdot b_h(x, x^i) \cdot y^i,$$

where β_i's are coefficients. If we estimate f as a locally weighted average, i.e., $\sum_{i=1}^{N} \beta_i b_h(x, x^i) = 1$, then $\beta_i = \frac{1}{\sum_{j=1}^{N} b_h(x, x^j)}, j = 1, ..., N$ and the estimator becomes

$$\hat{f}(x) = \sum_{i=1}^{N} \frac{b_h(x, x^i)}{\sum_{j=1}^{N} b_h(x, x^j)} \cdot y^i,$$

which is the well-known **Nataraya-Watson kernel estimator**.[5] In this estimator (or regressor), $\hat{f}(x)$ is always a convex combination of y^i's and the weights are proportional

to $b_h(x, x^i)$.

Remark. The Nataraya-Watson estimator is biased if the density of X varies around x.

To alleviate the biased problems for kernel estimators, one can resort to a generalization of kernel regression called *local linear regression*. The procedures go as follows.

1. Given a *query point* x, compute the weight function $w_i = b_h(x, x^i)$ for all $i = 1, ..., N$.
2. Solve the **weighted sums of squares** $\min_{\beta,\beta_0} \sum_{i=1}^{N} w_i(y^i - \beta^T x^i - \beta_0)^2$ to obtain β, β_0 (β, β_0 depend on x through w_i).[‡]
3. Calculate $\hat{f}(x) = \beta^T x + \beta_0$.

Remark. The Nataraya-Watson estimator solves a local linear regression with fixed $\beta = 0$.

4.2 Kernel (Binary) Classification

Given the training data $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \{Class1, Class2\}, i = 1, ..., N\}$, we can encode the binary responses y^i's into $\{-1, 1\}$. Then the **kernel binary classifier** can be written as

$$\hat{f}(x) \propto \sum_{i=1}^{N} y^i \cdot b\left(\frac{x - x^i}{h}\right),$$

where b is a kernel function defined in Section 3. The prediction is based on the sign of $\hat{f}(x)$, i.e.,

$$y(x) = \begin{cases} 1 & \text{(or Class 1) if } \hat{f}(x) > 0, \\ -1 & \text{(or Class 2) if } \hat{f}(x) < 0. \end{cases}$$

The plug-in estimator $\{x \in \mathcal{R}^d : \hat{f}(x) = 0\}$ of the **solution manifold** $\{x \in \mathcal{R}^d : f(x) = 0\}$ is the decision boundary of the kernel classifier. In addition, the decision boundary for a kernel binary classifier can be viewed as a plug-in estimator of the density level-set at level 0, for which asymptotic properties and visualization techniques have been analyzed and proposed. See [7] for details.

5 K-D Trees & Ball Trees

Both K-Nearest-Neighbor and kernel prediction methods involve scanning the whole dataset for every single prediction. Given training data $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \mathcal{Y}, i = 1, ..., N\}$,

- for K-Nearest Neighbor, predicting $f(x)$ for a single new instance x involves computing N distances in a d-dimensional space. The computational cost is approximately $\mathcal{O}(Nd)$.

[‡]See section 5.4 in [5] for detailed calculation.

- for kernel methods, finding the data points within the support of the kernel function, usually a d-dim ball with radius r, also involves computing the distances of a single x to all training data points.

The neighbor search (or computing pairwise distances of training data points) is a polynomial-time process but still *computational expensive*, especially when the dimension d is high. Can we design some algorithms that are more efficient?
The answer is **Yes**, if we index (i.e. preprocess) the training data. Indexing here means organizing the data in a way that makes finding the neighbors of any given point fast. In particular, with indexing, searching neighbors of a given point x *does not require comparing* x *with all* N *data points.*
The examples of indexing methods include,

- K-D trees
- Ball trees
- A-D trees (for discrete data)
- Locality Sensitive Hashing
- ... (many other methods with guarantees)

5.1 K-D Trees

A **K-D tree** (short for k-dimensional tree) is a binary tree whose leaf nodes are k-dimensional points and every non-leaf node corresponds to an implicit partition of the data space into two hyper-rectangular regions. Given a data set $\mathcal{D} = \{(x^i, y^i) \in \mathbb{R}^d \times \mathcal{Y}, i = 1, ..., N\}$ (y^i's would not be used in the tree construction), each node j stores:

- a subset of the data $\mathcal{D}_j \subset \mathcal{D}$
- a d-dimensional rectangle with $R_j = (r_{j,\min}, r_{j,\max}), j = 1, ..., d$, where $r_{j,\min} = \min_{\mathcal{D}_j} x_j^i, r_{j,\max} = \max_{\mathcal{D}_j} x_j^i$
- other statistics of $\mathcal{D}_j$, such as the number of nodes, mean, median, variance, etc.

Since there are many possible ways to choose axis-aligned splitting planes, there exist many different ways to construct a K-D tree for any given data set. Algorithm 1 illustrates a version of K-D tree construction in which the longest dimension of R_j would be split.

Figure 3a shows an example of KD trees and construction procedures. If a **balanced** K-D tree (i.e., the maximal number of levels below the root is as small as possible) is required, one can cycle through the axes used to select the splitting planes. For example, in a 3-dimensional tree, the root would have an x-aligned plane, the root's children would both have y-aligned planes, the root's grandchildren would all have z-aligned planes, the root's great-grandchildren would all have x-aligned planes, the root's great-great-grandchildren would all have y-aligned planes, and so on.[8]

5.2 Nearest Neighbor Search via K-D Tree

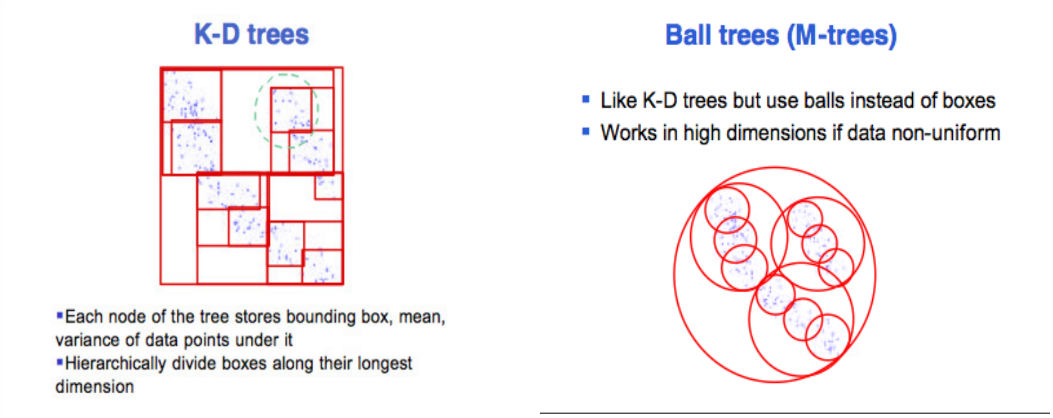
The nearest neighbour search algorithm aims to find the point in the data set that is nearest to a given query point. This search can be done efficiently by using the tree properties to quickly eliminate large portions of the search space.[9]

Algorithm 1 K-D Tree Construction

Input: (labeled) training set $\mathcal{D}$ (labels are not used in the tree construction)
Initialize the tree root R_0 with $\mathcal{D}_0 = \mathcal{D}$
while Leaf nodes can be split **do**
Choose a leaf node j with $|\mathcal{D}_j| > N_0$ points (N_0 is a threshold)

1. Find the longest dimension of R_j, i.e., $k = \arg\max_{j=1,\ldots,d}(r_{j,\max} - r_{j,\min})$ and set $r = (r_{k,\max} - r_{k,\min})/2$.
2. Split $\mathcal{D}_j$ into $\mathcal{D}_{j,left}$ and $\mathcal{D}_{j,right}$ with $x^i \in \mathcal{D}_{j,left}$ iff $x^i_k \leq r, x^i_k \in \mathcal{D}_j$.
3. Create new leaves $R_{j,left}, R_{j,right}$ storing $\mathcal{D}_{j,left}, \mathcal{D}_{j,right}$ and their respective bounding boxes and other statistics.

end while



(a) A K-D Tree and Construction Procedures (b) An Example of Ball Trees

Figure 3: K-D Trees and Ball Trees

Given a query point x, a search radius r, and a data set $\mathcal{D}$ indexed by a K-D tree $\mathcal{T}$, we aim to find all the points in $\mathcal{D}$ that are in the ball $B_x(r) = \{x^i \in \mathcal{D} : ||x^i - x|| \leq r\}$ (i.e., the r-neighbors of x).
The efficiency of nearest neighbor search via K-D trees is guaranteed by the following observations:

- Checking if $B_x(r)$ intersects with a hyper-rectangle R is fast. $\implies$ If $B_x(r) \cap R = \emptyset$, then no data points in R can be neighbors of x.
- Checking if $B_x(r)$ contains a hyper-rectangle R is fast. A naive algorithm is to compute the distances of all the vertices to x and check whether they are all $\leq r$. $\implies$ If $B_x(r) \supset R$, then all data points in R are neighbors.

Algorithm 2 presents a way to retrieve nearest neighbors of a query point x via a pre-constructed K-D tree.

Nearest-Neighbor search via K-D trees may exhibit inefficiency when the data dimension d is large, since the data points are far away from each other in high dimensional

Algorithm 2 K-D Tree Neighbors Retrieval Algorithm

Input: $(x, r, \mathcal{T})$, where x is a query point, r is a search distance, and $\mathcal{T}$ is a K-D tree.
Initialize the set of neighbors $N_r = \emptyset$, $R = root(\mathcal{T})$
Call the function ProcessNode(x, r, R, N_r) recursively

ProcessNode(x, r, R, N_r):
if $B_x(r) \cap R_j = \emptyset$ **then**
    return
else if $B_x(r) \supset R_j$ **then**
    $N_r \leftarrow N_r \cup R_j$
    return
else if R_j is a leaf **then**
    for $x^i \in \mathcal{D}_j$, if $||x - x^i|| \leq r, N_r \leftarrow N_r \cup \{x^i\}$
    return
else
    call ProcessNode$(x, r, R_{j,left}, N_r)$
    call ProcessNode$(x, r, R_{j,right}, N_r)$
    return
end if

space. In this case, most of the points in the tree will be evaluated and nearest-neighbor search via K-D trees will end up being a needlessly fancy brute search. One remedy to this issue is to construct **Ball Trees**, where every node defines a d-dimensional ball containing a subset of the points to be searched. Several existing ball tree construction algorithms are available at [10]. Figure 3b shows an example of ball trees.

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