Lecture 4: K-means and K-nearest neighbors

Reading: Sections 13.3, 14.3.6

GU4241/GR5241 Statistical Machine Learning

Linxi Liu
January 26, 2018

Clustering

We assign a class to each sample in the data matrix. However, the class *is not an output variable*; we only use input variables.

Clustering is an **unsupervised** procedure, whose goal is to find homogeneous subgroups among the observations. It has wide applications in practice. Image segmentation, handwritten digit identification, vector quantization

We will discuss 4 algorithms in this semester:

- K-means clustering
- K-medoids clustering
- Hierarchical clustering
- EM algorithm

Handwritten digit identification

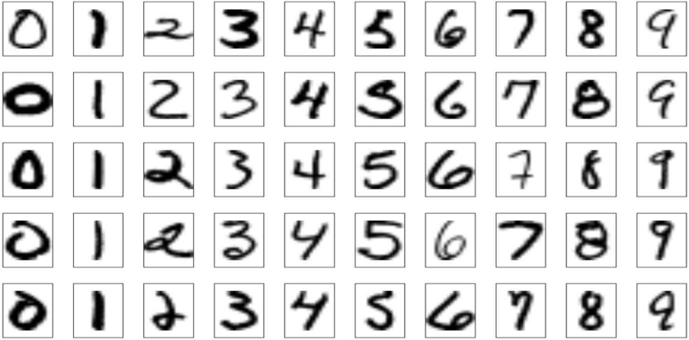
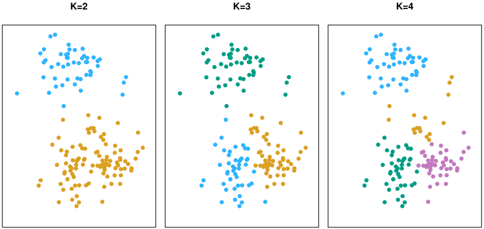


FIGURE 11.9. *Examples of training cases from ZIP code data. Each image is a* 16×16 8-*bit grayscale representation of a handwritten digit.*

Image segmentation

K-means clustering

- K is the number of clusters and must be fixed in advance.



ISL Figure 10.5

- The goal of this method is to maximize the similarity of samples within each cluster:

$$\min_C W(C) \quad ; \quad W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} d(x_i, x_j).$$

K-means clustering algorithm

1. Assign each sample to a cluster from 1 to K arbitrarily, e.g. at random.

2. Iterate these two steps until the clustering is constant:

   - Find the *centroid* of each cluster ℓ; i.e. the average $\overline{x}_{\ell,:}$ of all the samples in the cluster:

   $$\overline{x}_{\ell,j} = \frac{1}{|\{i : C(i) = \ell\}|} \sum_{i:C(i)=\ell} x_{i,j} \quad \text{for } j = 1, \ldots, p.$$

   - Reassign each sample to the nearest centroid.

K-means clustering algorithm

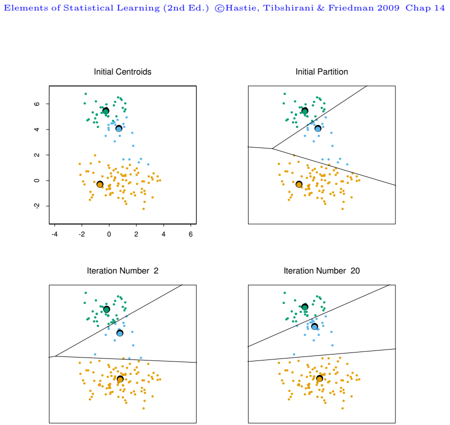


FIGURE 14.6. *Successive iterations of the K-means clustering algorithm for the simulated data of Figure 14.4.*

Properties of K-means clustering

- The algorithm always converges to a local minimum of

$$\min_C W(C) \quad ; \quad W(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(j)=k} d(x_i, x_j).$$

Why? When d is the Euclidean distance

$$\frac{1}{2}\sum_{C(i)=\ell}\sum_{C(j)=\ell} d(x_i, x_j) = |N_\ell| \sum_{C(i)=\ell} d(x_i, \overline{x}_\ell)$$

Properties of K-means clustering

- The algorithm always converges to a local minimum of

$$\min_C W(C) \quad ; \quad W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} d(x_i, x_j).$$

Why? When d is the Euclidean distance

$$\frac{1}{2} \sum_{C(i)=\ell} \sum_{C(j)=\ell} d(x_i, x_j) = |N_\ell| \sum_{C(i)=\ell} d(x_i, \overline{x}_\ell)$$

This side can only be reduced in each iteration.

- Each initialization could yield a different minimum.

Example: K-means output with different initializations

ISL Figure 10.7

In practice, we start from many random initializations and choose the output which minimizes the objective function.

Practical Issues

- Categorical features are usually coded as dummy variables:

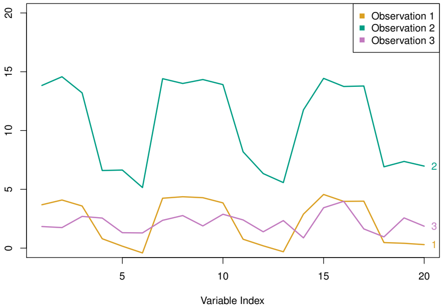
$$X = 1, 2, \text{ or } 3 \quad \rightarrow \quad \begin{array}{r} (1\ 0\ 0) \\ (0\ 1\ 0) \\ \text{or} \quad (0\ 0\ 1) \end{array}$$

- Weighting is also possible

- How to choose the number of clusters K?

Correlation distance

- Euclidean distance would cluster all customers who purchase few things (orange and purple).
- Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.



Fact of correlation distance

Correlation is defined by

$$\rho(x_i, x_{i'}) = \frac{\sum_j (x_{ij} - \bar{x}_i)(x_{i'j} - \bar{x}_{i'})}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2 \sum_j (x_{i'j} - \bar{x}_{i'})^2}},$$

where $\bar{x}_i$ = mean of obeservation i.

If observations are standardized:

$$x_{ij} \leftarrow \frac{x_{ij} - \bar{x}_i}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2}},$$

then $2(1 - \rho(x_i, x_{i'})) = \sum_j (x_{ij} - x_{i'j}))^2$.

K-medoids clustering

1. Assign each sample to a cluster from 1 to K arbitrarily, e.g. at random.

2. Iterate these two steps until the clustering is constant:

   - For a given cluster assignment C find the observation in the cluster minimizing total pairwise distance with the other cluster members:

     $$i_k^* = \underset{\{i:C(i)=k\}}{\operatorname{argmin}} \sum_{C(i')=k} d(x_i, x_{i'}).$$

     Then $z_k = x_{i_k^*}$, $k = 1, 2, \ldots, K$ are the current estimates of the cluster centers.

   - Given a current set of cluster centers $\{z_1, \ldots, z_K\}$, minimize the total error by assigning each observation to the closest (current) cluster center:

     $$C(i) = \underset{1 \leq k \leq K}{\operatorname{argmin}}\, d(x_i, z_k).$$

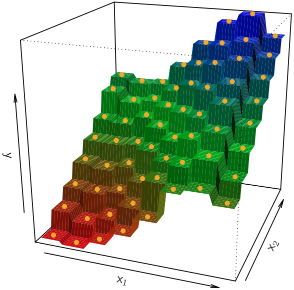
K-medoids clustering

- Same as K-means, except that centroid is required to be one of the observations.
- Advantage: centroid is one of the observations— useful, for example when features are 0 or 1. Also, one only needs pairwise ditances for K-medoids rather than the raw observations.

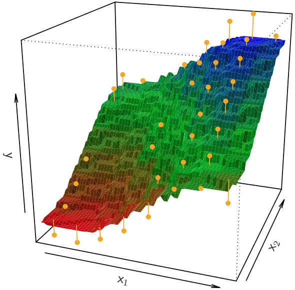
K-nearest neighbors regression

KNN regression: prototypical nonparametric method.
Given a training set $(\mathbf{X}, \mathbf{y})$:

$$\hat{f}(x) = \frac{1}{K} \sum_{i \in N_K(x)} y_i$$

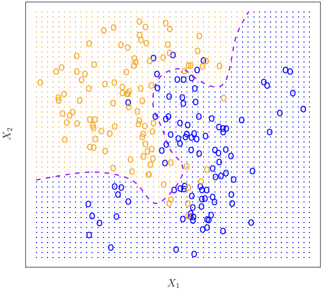


$K = 1$



$K = 9$

Classification problem



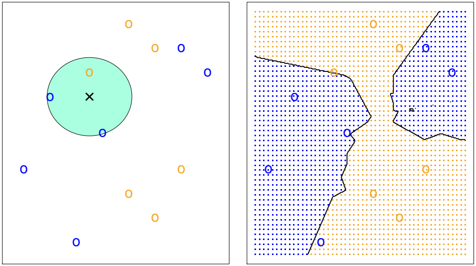
ISL Figure 2.13

Recall:

- $X = (X_1, X_2)$ are inputs.
- Color $Y \in \{\text{Yellow}\ , \text{Blue}\}$ is the output.
- (X, Y) have a joint distribution.
- Purple line is *Bayes boundary* — the best we could do if we knew the joint distribution of (X, Y)

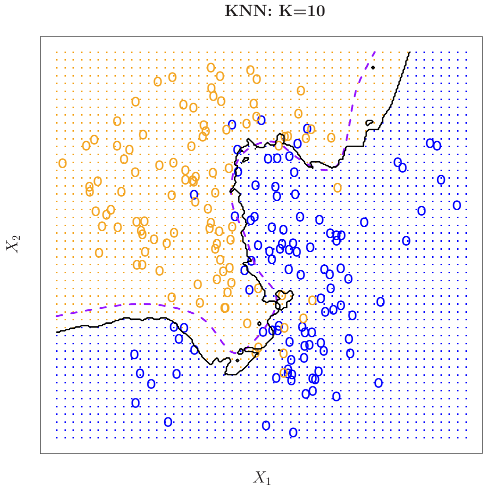
K-nearest neighbors

To assign a color to the input $\times$, we look at its $K = 3$ nearest neighbors. We predict the color of the majority of the neighbors.



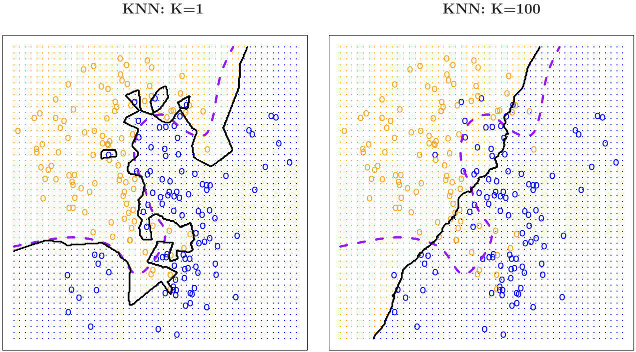
ISL Figure 2.14

K-nearest neighbors also has a decision boundary



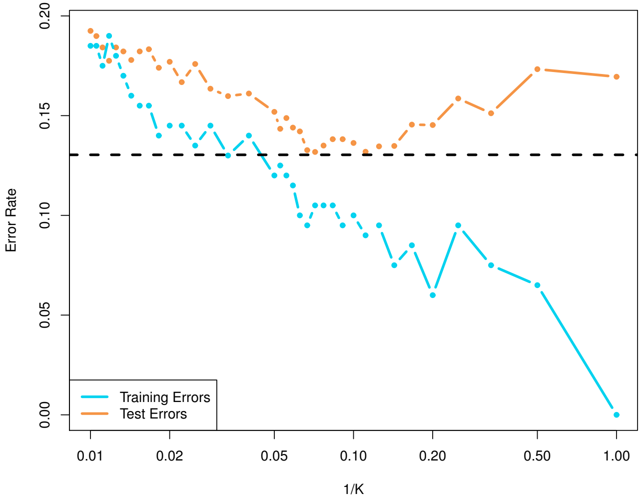
ISL Figure 2.15

The higher K, the smoother the decision boundary



ISL Figure 2.16

Test error vs. training error



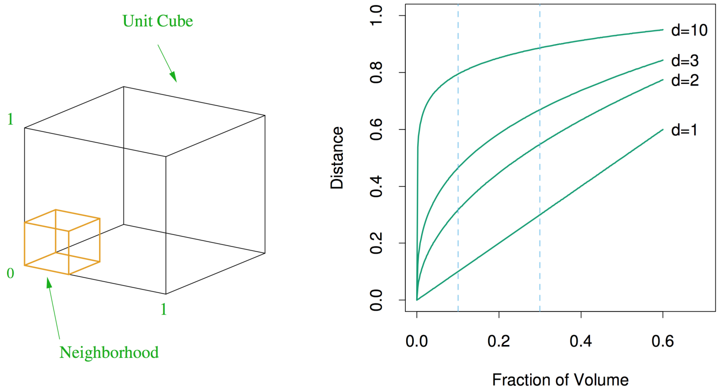
ISL Figure 2.17

Curse of dimensionality

K-nearest neighbors can fail in high dimensions, because it becomes difficult to gather K observations close to a target point x_0:

- near neighborhoods tend to be spatially large, the estimates are biased.
- reducing the spatial size of the neighborhood means reducing K, and the variance of the estimate increases.

Curse of dimensionality



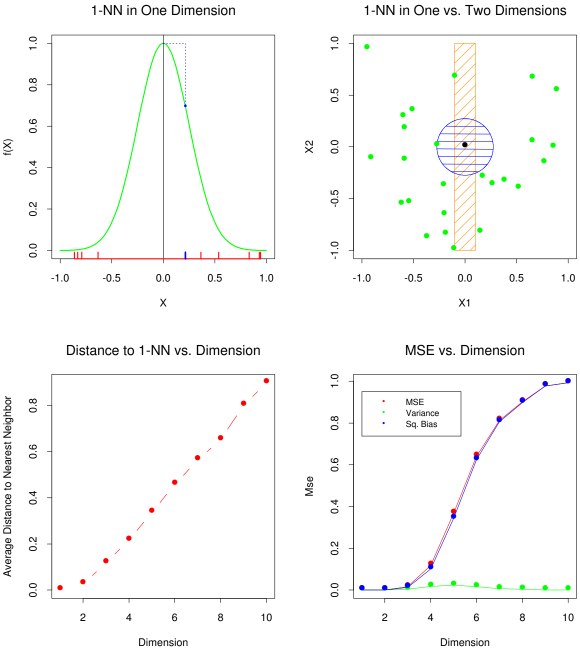
ESL Figure 2.6

- We want to obtain a hypercubical neighborhood about a target point to capture a fraction r of the observations.
- The expected edge length will be $e_p(r) = r^{1/p}$. In ten dimensions, $e_{10}(0.01) = 63\%$.

Example

- 1000 training examples x_i generated uniformly on $[-1, 1]^p$.
- $Y = f(X) = e^{-8\|X\|^2}$ (no measurement error).
- use the 1-nearest-neighbor rule to predict y_0 at the test-point $x_0 = 0$.

$$\begin{aligned} \mathsf{MSE}(x_0) &= \mathbb{E}_{\mathcal{T}}[f(x_0) - \hat{y}_0]^2 \\ &= \mathbb{E}_{\mathcal{T}}[\hat{y}_0 - \mathbb{E}_{\mathcal{T}}(\hat{y}_0)]^2 + [\mathbb{E}_{\mathcal{T}}(\hat{y}_0) - f(x_0)]^2 \\ &= \mathsf{Var}_{\mathcal{T}}(\hat{y}_0) + \mathsf{Bias}^2(\hat{y}_0). \end{aligned}$$


1-NN in One Dimension
f(X)
X
1-NN in One vs. Two Dimensions
X2
X1
Distance to 1-NN vs. Dimension
Average Distance to Nearest Neighbor
Dimension
MSE vs. Dimension
Mse
Dimension
MSE
Variance
Sq. Bias

An example when the variance dominates

Assume the regression function is: $f(X) = \frac{1}{2}(X_1 + 1)^3$.