Nearest Neighbors Methods

Review: Types of Classifiers

- **A classifier is a function that assigns to a sample, $\mathbf{x}$ a class label $\hat{y}$**

$$\hat{y} = f(\mathbf{x})$$

- **A probabilistic classifier obtains conditional distributions $\Pr(Y|\mathbf{x})$, meaning that for a given $\mathbf{x} \in \boldsymbol{X}$, they assign probabilities to all $y \in Y$**
  - Hard classification

$$\hat{y} = \arg\max_{y} \Pr(Y = y|\,\mathbf{x})$$

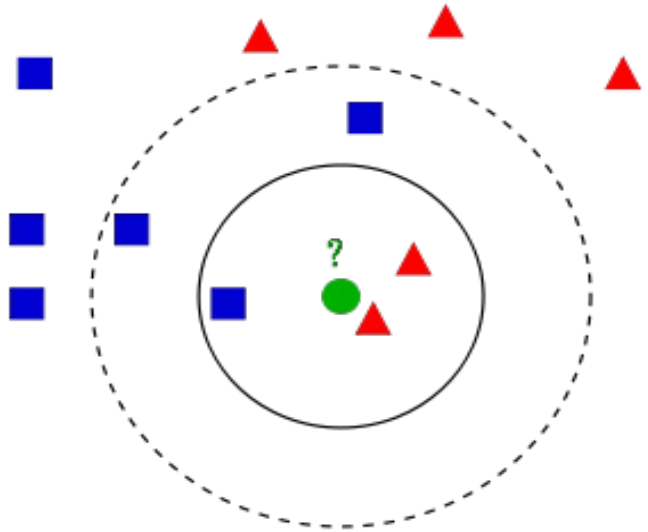
Any other classifiers not belonging to a probabilistic approach?

k-Nearest Neighbor

k-Nearest Neighbors(kNN)

- **Nonparametric method used for classification and regression**

- **For classification**
  - Output class of data sample is determined by output class of its k-nearest neighbors
  - Majority vote
    - ✓ assign the output class to the most common class among k-nearest neighbors



- **For regression**
  - Output value of data sample is determined by output value of its k-nearest neighbors of the data sample
  - Output value is the average value of k-nearest neighbors
    - ✓ There are several different ways to calculate average

※ What is Nonparametric Method

- **Parametric**
  - Assume that data are drawn from a specific form of function up to unknown parameters
    - ✓ Linear regression, logistic regression

- **Nonparametric**
  - Assume that data are drawn from a certain unspecified function
  - Unlike parametric methods, there is no single global model
  - Learn to find patterns from training set and interpolate
  - Heavier computational cost than parametric ones

Distance Measure

- **Distance is a numerical description of how far apart objects are**
  - Euclidean distance, one of distance measures, is common
    - ✓ Euclidean distance of two-dimensional data points, $(x_1, y_1), (x_2, y_2)$

$$d = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

    - ✓ In general, Euclidean distance of two data points, $(x_1, x_2, , \dots, x_n), (y_1, y_2, \dots, y_n) \in \mathbb{R}^n$

$$d = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \cdots + (x_n - y_n)^2}$$

- **Other distance measures**
  - 1-norm distance(Manhattan distance)

$$\sum_i^n |x_i - y_i|$$

  - p-norm distance (when p=2→ Euclidean distance)

$$\left(\sum_i^n (x_i - y_i)^p\right)^{1/p}$$

Distance Measure

- **Distance measure should hold the following**
  - $d(x, y) \geq 0$
    - ✓ Non-negativity
  - $d(x, y) = 0 \Leftrightarrow x = y$
    - ✓ Identity of indiscernibles
  - $d(x, y) = d(y, x)$
    - ✓ *symmetry*
  - $d(x, z) \leq d(x, y) + d(y, z)$
    - ✓ Subaddivity or triangle inequality

Distance Measure

- **What if variables are not numerical**
  - Other metrics are required for categorical variables

- **Metrics for categorical variables**
  - Hamming distance

$$d(x, y) = \frac{\sum_i I(x_i \neq y_i)}{\dim(x)}$$

  - ✓ $I(x_i \neq y_i)$ is 1 if and only if $x_i \neq y_i$
  - ✓ $\dim(x)$ is the dimension of x

Distance Measure

- **Metrics for categorical variables**
  - Jaccard distance
    - ✓ Used to calculate the distance between binary vectors

		y	
		0	1
x	0	a	b
	1	c	d

- ✓ a: the total number of attributes where x and y both have a value of 0
- ✓ b: the total number of attributes where the attribute of x is 0 and the attribute of y is 1
- ✓ c: the total number of attributes where the attribute of x is 1 and the attribute of y is 0
- ✓ d: the total number of attributes where x and y both have a value of 1

$$d(x, y) = \frac{b + c}{b + c + d}$$

Question

- **Find k-nearest neighbors based on given data points**

1) Find k-nearest neighbors of 5th objects when k=3 using Euclidean distance

2) Find k-nearest neighbors of 5th objects when k=3 using Manhattan distance

index	x	y
1	1	1
2	2	3
3	4	6
4	3	1
5	2	4
6	4	0
7	7	5
8	6	2

Feature Scaling

- **Scale of variable affects on determination of nearest neighbors**

- **Which sample is the nearest neighbor of data sample 1?**

i	x_1	x_2	x_3	x_4	y
1	9	30	100	0.5	1
2	9	25	250	0.1	0
3	9	44	220	0.7	0
4	7.5	75	170	1.2	1
	…	…	…	…	…

i	**Distance from p_1**
1	-
2	150.0838
3	120.8141
4	83.23305
	…

- Scale of variable x_3 dominates over other variables
- The nearest neighbor is strongly dependent on x_3

It is unfair!

Normalization

- **Normalization is to adjust values of variables with different scales to common scale**
  - There are several different ways for normalization

- **Commonly used normalization method**

$$x \rightarrow \frac{x - \mu}{\sigma}$$

  - μ=mean value of the variable
  - σ=standard deviation of the variable
  - μ and σ are computed by sample data points

$$x \rightarrow \frac{x - x_{min}}{x_{max} - x_{min}}$$

  - x_{max} is the maximum value of variable x and x_{min} is the minimum value of variable x
  - Normalized value is within [0, 1]

Mahalanobis Distance

- **Normalization based on normal distribution($x \rightarrow \frac{x-\mu}{\sigma}$) assumes that the sample points are distributed about the center of mass in a spherical manner**
  - In real data, variables are correlated with other variables

Need to consider scale (level of spread along axis) and correlation to measure distance

Mahalonobis distance

Mahalanobis Distance

- **Mahalanobis distance**

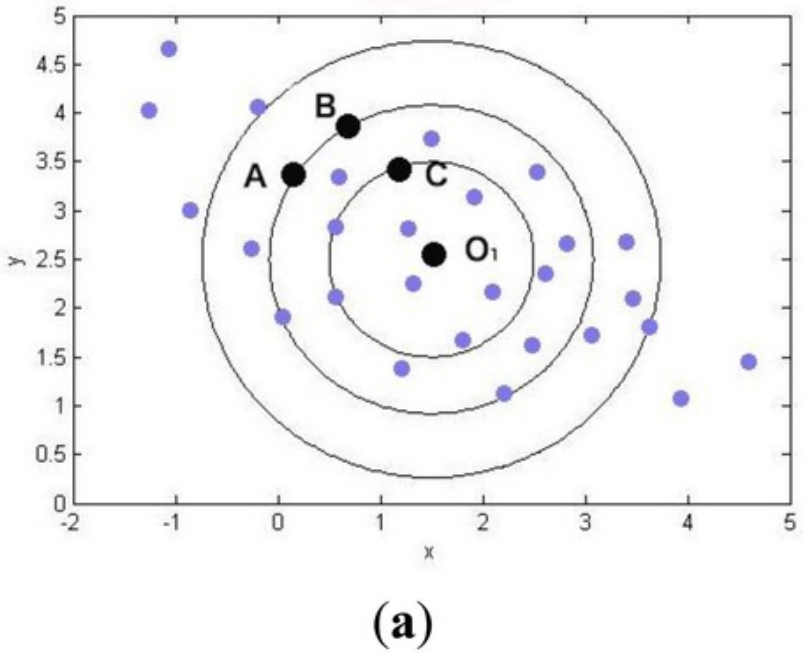
$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T S^{-1} (\mathbf{x}_1 - \mathbf{x}_2)}$$

  - S is sample covariance matrix
  - If covariance matrix is diagonal(no correlation), the resulting distance measure is as the same as the standardized distance

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{\sum_{i=1}^{p} \frac{(x_{1i} - x_{2i})^2}{s_i^2}}$$

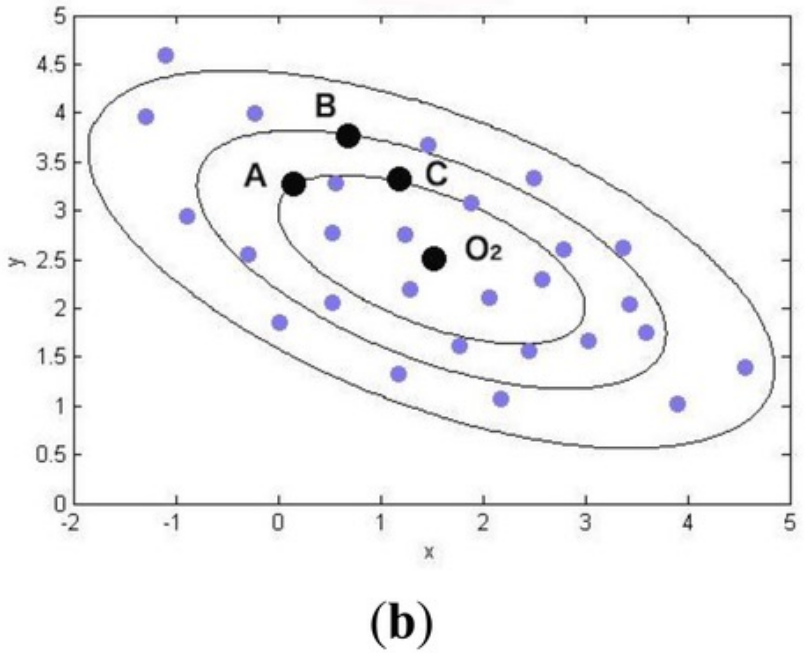
Mahalanobis Distance

- **Comparison between Euclidean distance and Mahalanobis distance**



(a)

Euclidean distance



(b)

Mahalanobis distance

Procedure of k-NN

Decide the number of nearest neighbors k and distance measure

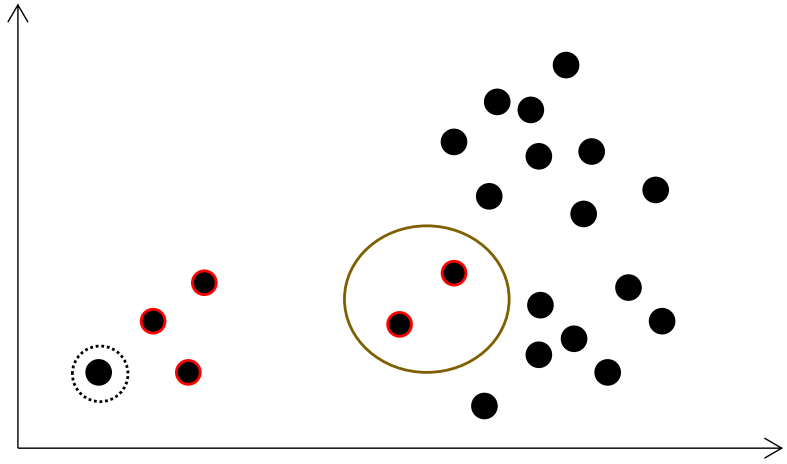
For all data point in test set, find k nearest neighbors

Obtain output value based on output values of neighbors

Fixed-radius Nearest Neighbors

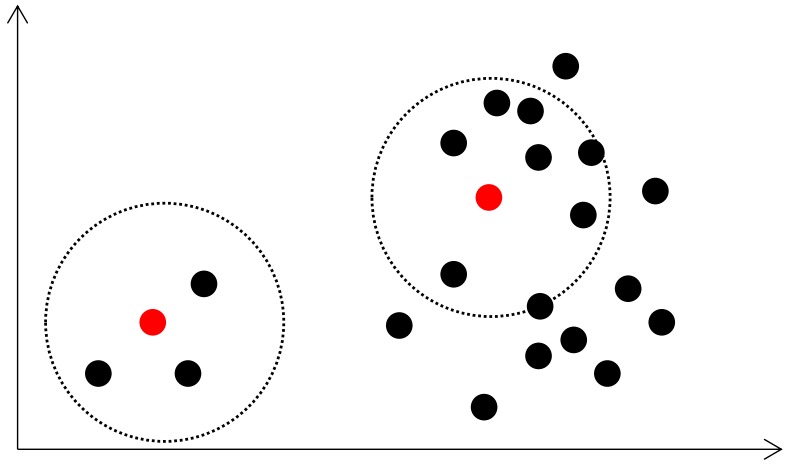
Problem of Fixed-Number of Nearest Neighbors

- **When distribution of data set is not homogenous, samples not similar to data point x can be obtained in the nearest neighbors**
  - $k = 5$



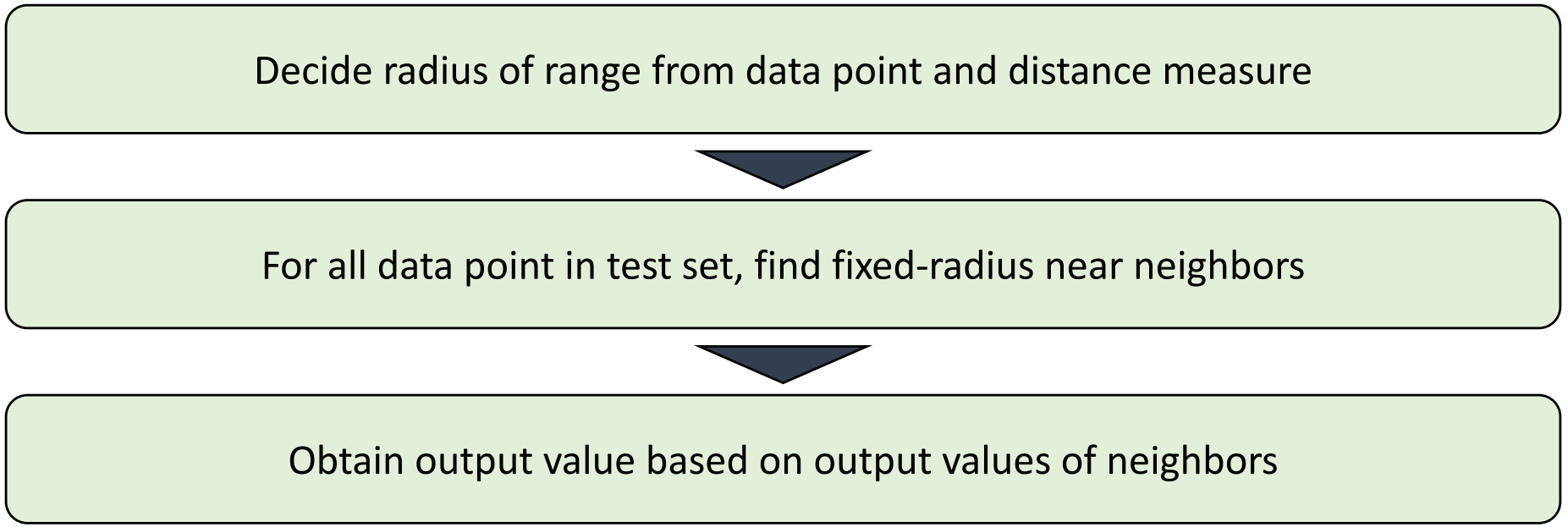
Fixed-Radius Near Neighbors

- **Fixed-radius near neighbors are neighbors within fixed range from data point x**
  - Because of that, the number of neighbors may be different depending on the location



Fixed-Radius Near Neighbors Methods

- **The only difference of fixed-radius NN from kNN is the method to find the nearest neighbors**
  - Remained steps of classification and regression are the same



Thank you!