Two Simple ML Algorithms [1]

Shaobo Li

University of Kansas

[1] Partially based on Hastie, et al. (2009) ESL, and James, et al. (2013) ISLR

Clustering – an unsupervised learning method

- Goal: find subgroups of a sample observations
  - Not based on any single variable (e.g. gender, race)
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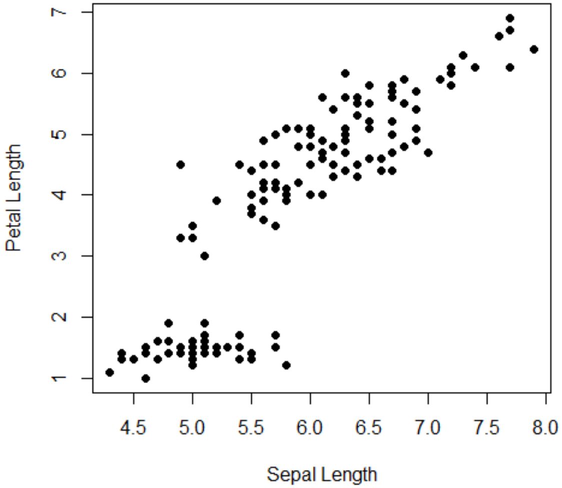
- The number of subgroup is subjective
- Approaches:
  - K-means clustering
  - Hierarchical clustering
  - Model-based clustering

An example – Iris data



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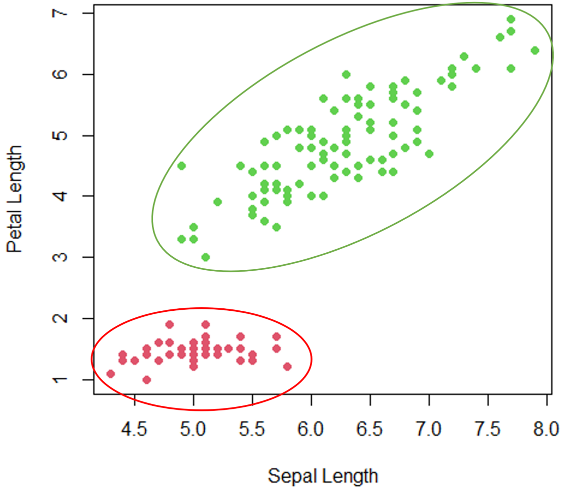

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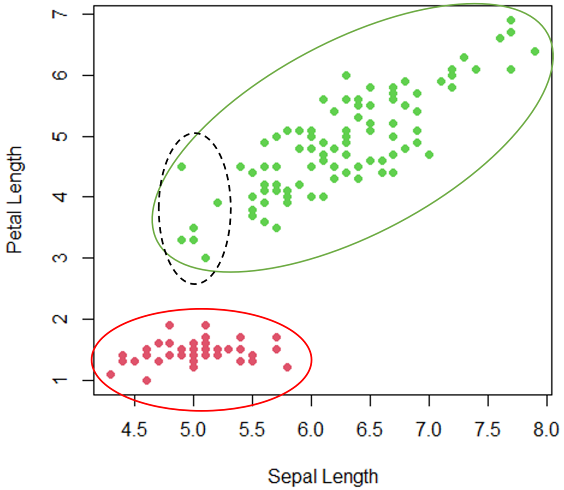


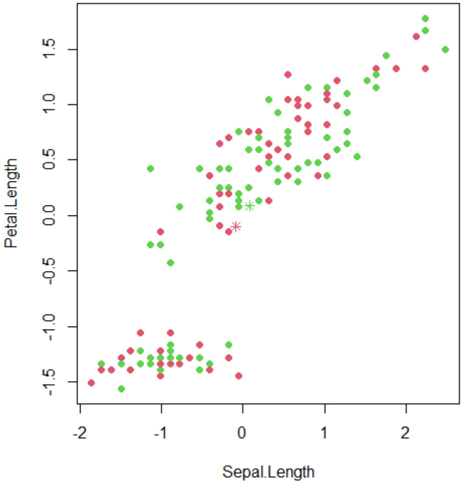
K-means clustering – step-by-step

Run the following R code, and see what it does.

```
iris1 <- scale(iris[,-c(2,4,5)])
n <- nrow(iris1)
index <- sample(2, n, replace = T)
iris.sub1 <- iris1[index==1,]
iris.sub2 <- iris1[index==2,]
mean.sub1 <- apply(iris.sub1, 2, mean)
mean.sub2 <- apply(iris.sub2, 2, mean)

plot(iris1, col=index+1, pch=16)
points(x=mean.sub1[1], y=mean.sub1[2], col=2, pch=8)
points(x=mean.sub2[1], y=mean.sub2[2], col=3, pch=8)
```

This is a random grouping (first step)



The next step

Run the following R code, and see what it does.

```
Eudist <- function(x, y) sqrt(sum((x-y)^2))

d1<-sapply(1:n,function(i) Eudist(mean.sub1,iris1[i,]))
d2<-sapply(1:n,function(i) Eudist(mean.sub2,iris1[i,]))
index.new <- apply(cbind(d1, d2), 1, which.min)
iris.sub1 <- iris1[index.new==1,]
iris.sub2 <- iris1[index.new==2,]
mean.sub1 <- apply(iris.sub1, 2, mean)
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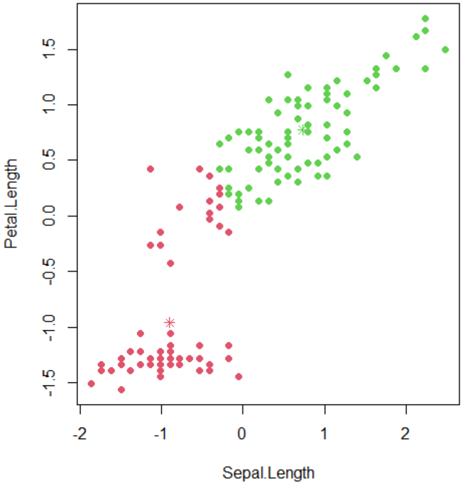
```

Data points are regrouped (second step)



How does this happen?

Let’s repeat the second step

```
d1<-sapply(1:n,function(i) Eudist(mean.sub1,iris1[i,]))
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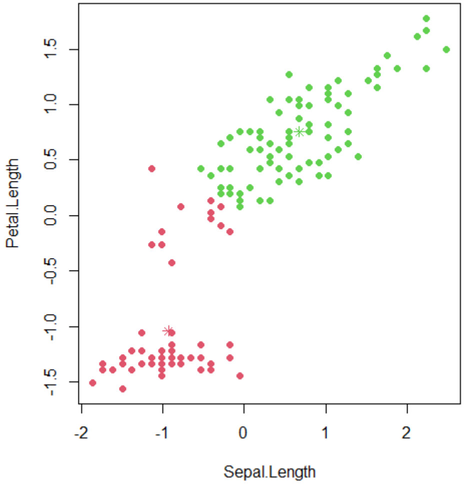
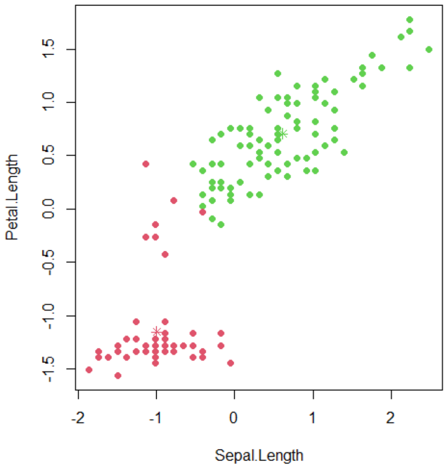
points(x=mean.sub2[1], y=mean.sub2[2], col=3, pch=8)
```

Note that the code does not change at all. Why?

Data points are regrouped again



We can keep repeating this step, until...



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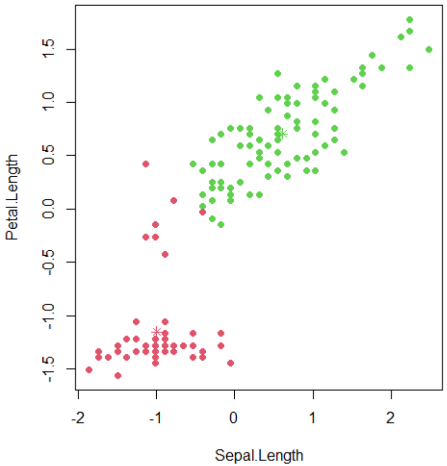

Members in each cluster do not change, which means the algorithm converges. How can we translate it into some numeric scores?

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- Sum of WSS across all clusters: total within-group sum squared error (TWSS)
- $SST - TWSS$: Between-group sum square
- Exercise:

  Revisit the algorithm we just performed. Compute the above three measures at the end of each step. How are they changing over iterations?

Choosing K

- Balancing the tradeoff between model complexity versus goodness of fit
  - Larger $K \implies$ higher complexity (poor interpretability) and better fit (maybe overfitting)
  - Smaller $K \implies$ lower complexity (better interpretability) and less precise
- A common approach to find optimal K: Elbow Method

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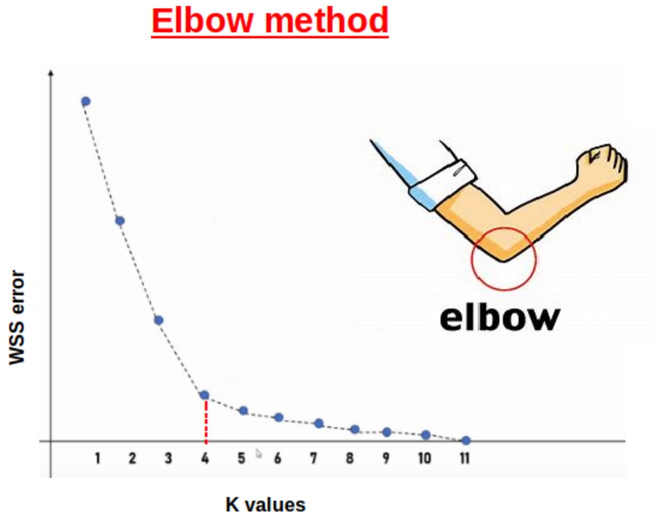
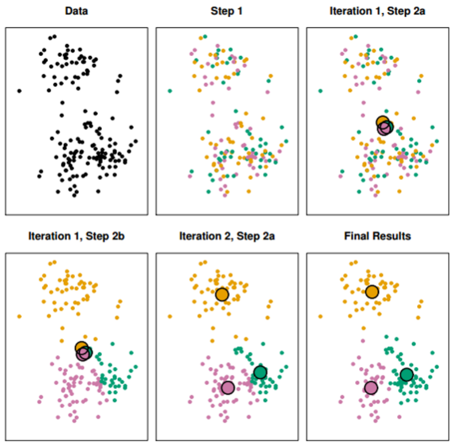
- A common approach to find optimal K: Elbow Method
  Plot TWSS vs. K and look for the "elbow" where additional clusters provide diminishing returns in variance reduction.

Elbow method



K-means algorithm recap



- Here is a very good animation to illustrate k-means clustering algorithm. [link]

K-means algorithm recap

1. Randomly find k data points (observations) as the initial centers
2. For each data point, find the closest center and label it (e.g., using different colors). Now you have k clusters
3. Re-calculate the centers of current clusters
4. Repeat step 2 and 3 until the centers do not change

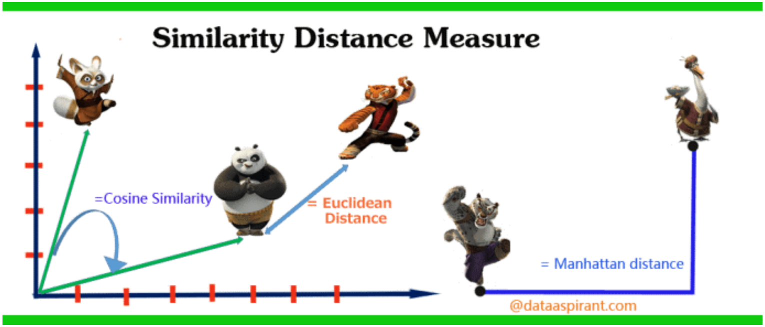
K-nearest neighbor (KNN)

- Model:

$$\hat{Y} = \hat{f}(\mathbf{x}) = \frac{1}{k} \sum_{\mathbf{x}_i \in N_k(\mathbf{x})} y_i$$

  where $N_k(\mathbf{x})$ is the neighborhood of $\mathbf{x}$ defined by the k closest points $\mathbf{x}_i$.
- The prediction $\hat{Y}$ is typically the majority vote (or average if Y is numeric) of the outcomes in the neighbor.
- k: size of the neighbor
  - smaller or bigger neighbor is better?
- The key computation: find the neighbor of a given observation $\mathbf{x}$

Distance-based Similarity Measures



KNN algorithm illustration

Data preparation

```
iris.X <- scale(iris[,-5])
iris.Y <- iris[,5]
iris.train.X <- iris.X[1:148,]
iris.train.Y <- iris.Y[1:148]
iris.test.X <- iris.X[149:150,]
iris.test.Y <- iris.Y[149:150]
```

KNN algorithm illustration

Key component – computing distance

```
Eudist <- function(x, y){
  sqrt (sum((x-y)^2))
}

dist.vec <- rep(NA, nrow(iris.train.X))
for(i in 1:nrow(iris.train.X)){
  dist.vec[i] <- Eudist(iris.test.X[1,],
                        iris.train.X[i,])
}
```

KNN algorithm illustration

Find neighbor and make prediction

```
K <- 10
index.neighbor <- order(dist.vec)[1:K]
Y.neighbor <- iris.train.Y[index.neighbor]
freqY.neighbor <- table(Y.neighbor)
sort(freqY.neighbor, decreasing = T)
names(sort(freqY.neighbor, decreasing = T))[1]
```

KNN algorithm illustration

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```

Can you define a function, let's call it `majority_vote()`, to integrate the majority vote step? Then you can call the function to get the output in one step. Like the following:

```
majority_vote(Y.neighbor)
```

What is the impact of k – an example[2]

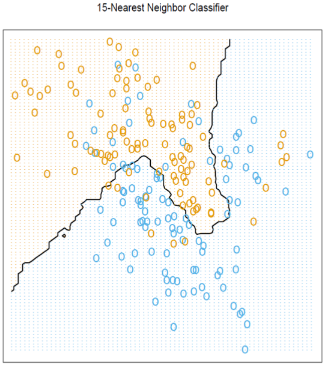

FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by 15-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the 15-nearest neighbors.*

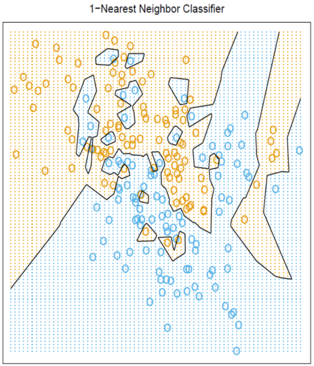

FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$), *and then predicted by 1-nearest-neighbor classification.*

[2]Source: ESL pp.15-16