20) K-Means Clustering and Hierarchical Clustering

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Reference

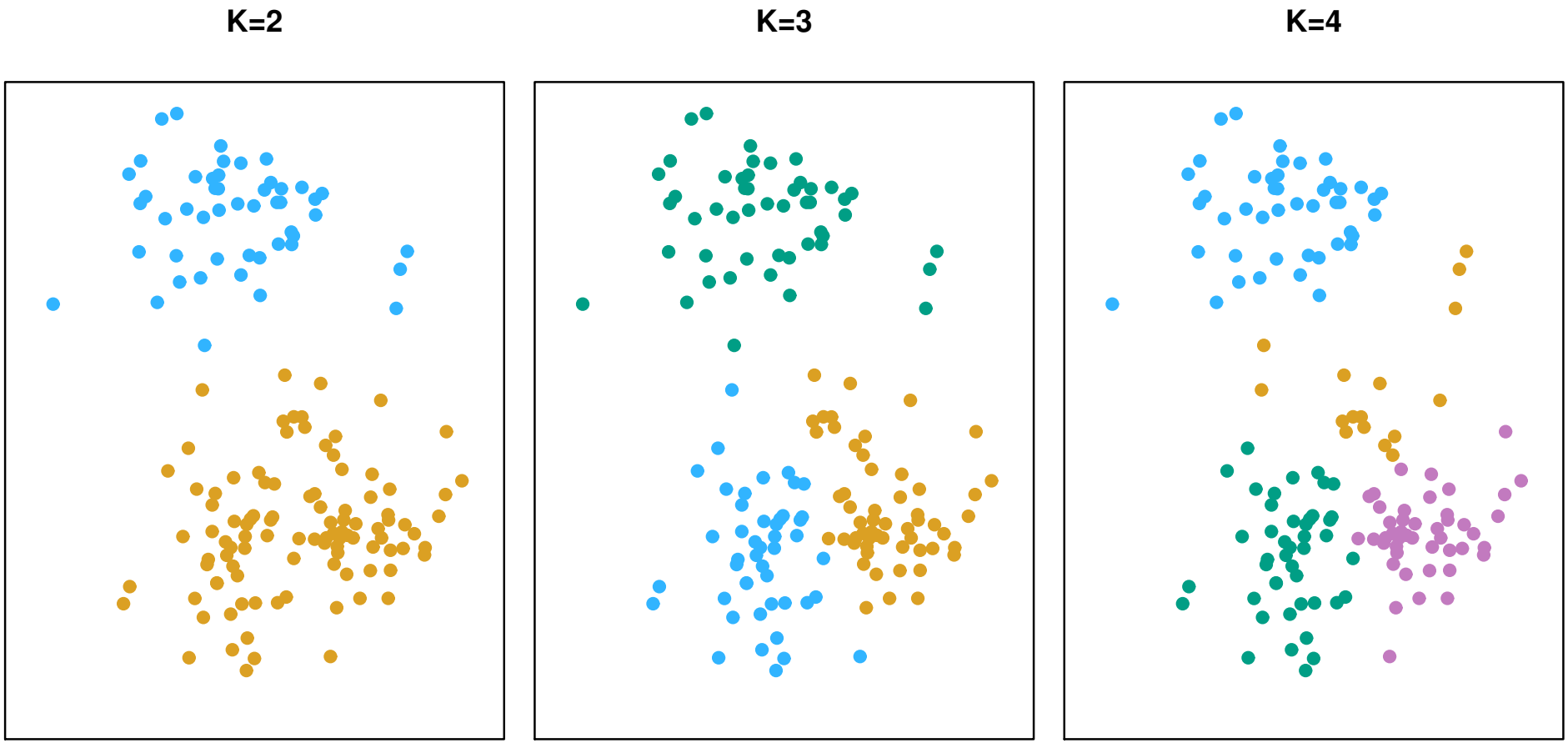
Tables, Graphics, and Figures from

An Introduction to Statistical Learning

James et al. (2017): Chapters: 10.3, 10.5, and 10.6

Hastie et al. (2017): Chapter: 14.3

Simulated Data Set with 150 Observations



K-Means Clustering

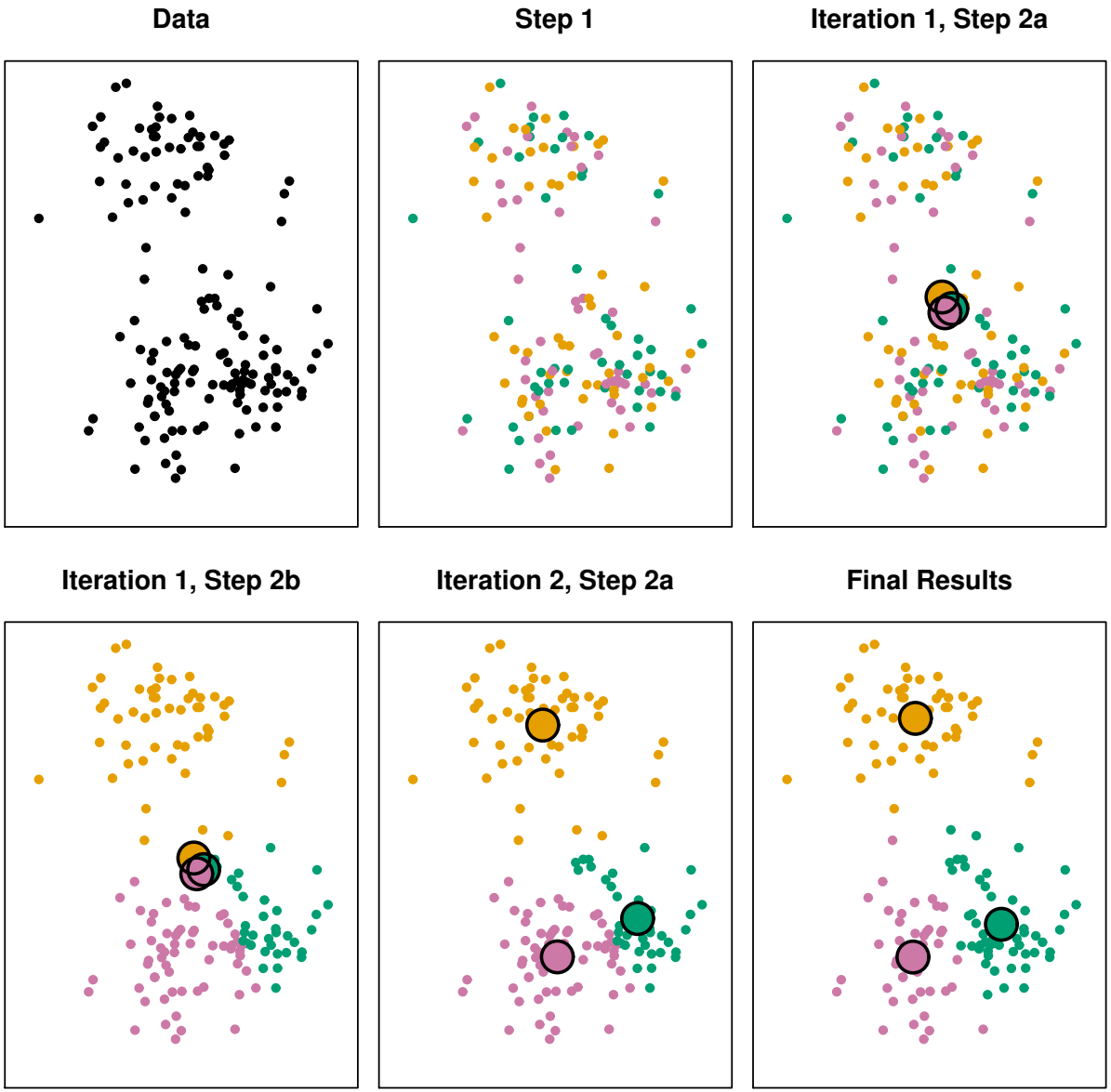
$$C_1 \cup C_2 \cup ... \cup C_K = \{1, ..., n\}$$

$$C_k \cap C_{k'} = \emptyset \text{ for all } k \neq k'$$

$$\underset{C_1,...,C_k}{Minimize}\{\sum_{k=1}^{K} W(C_k)\}$$

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

K-Means Clustering Algorithm



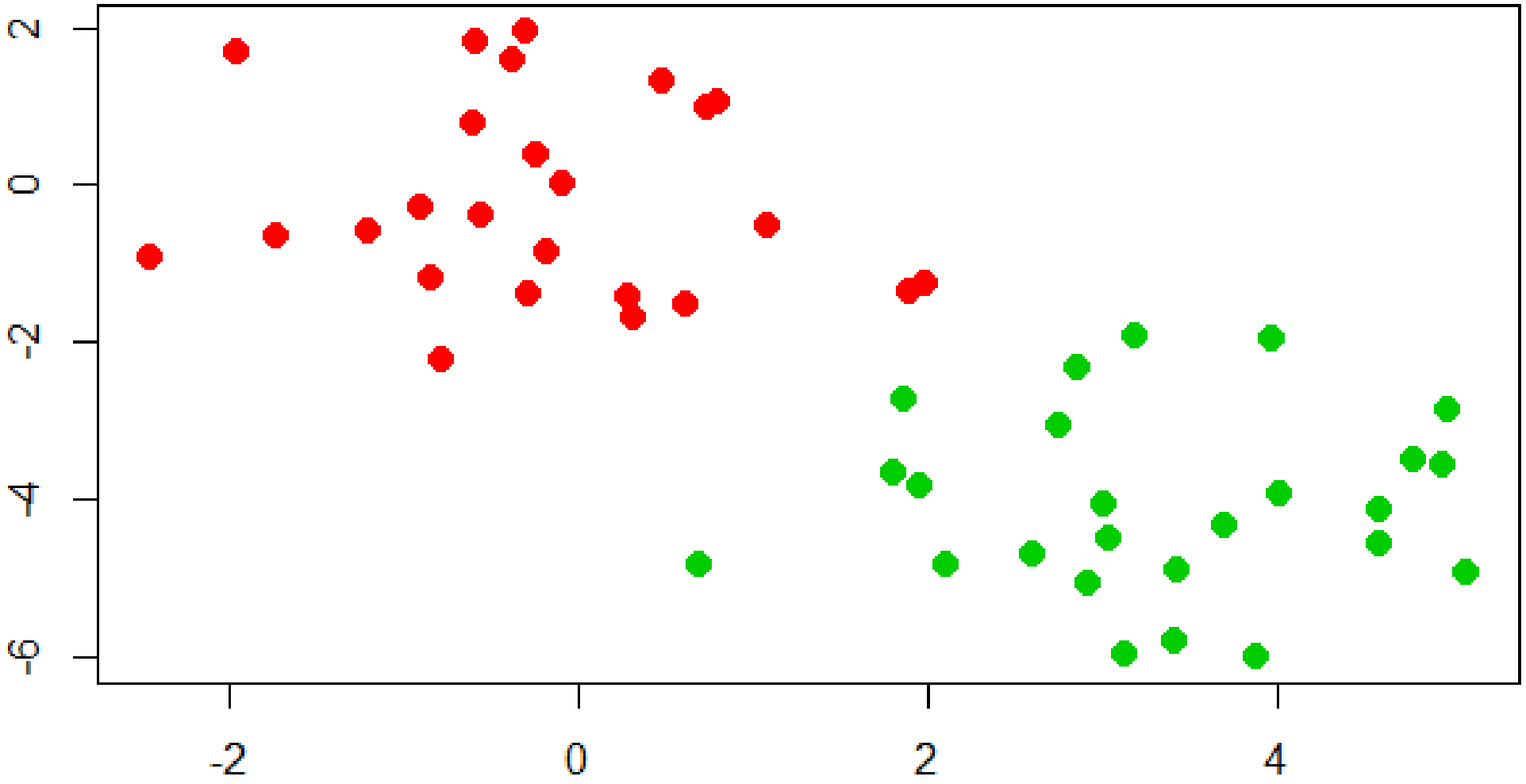
Different Random Assignment

set.seed(2)

```
x=matrix(rnorm(50*2), ncol=2)
x[1:25,1]=x[1:25,1]+3
x[1:25,2]=x[1:25,2]-4
km.out=kmeans(x,2,nstart=20)
km.out$cluster
```

```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
[26] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

plot(x, col=(km.out$cluster+1), xlab="", ylab="", pch=20, cex=2)



set.seed(4); km.out=kmeans(x,3,nstart=20)

km.out

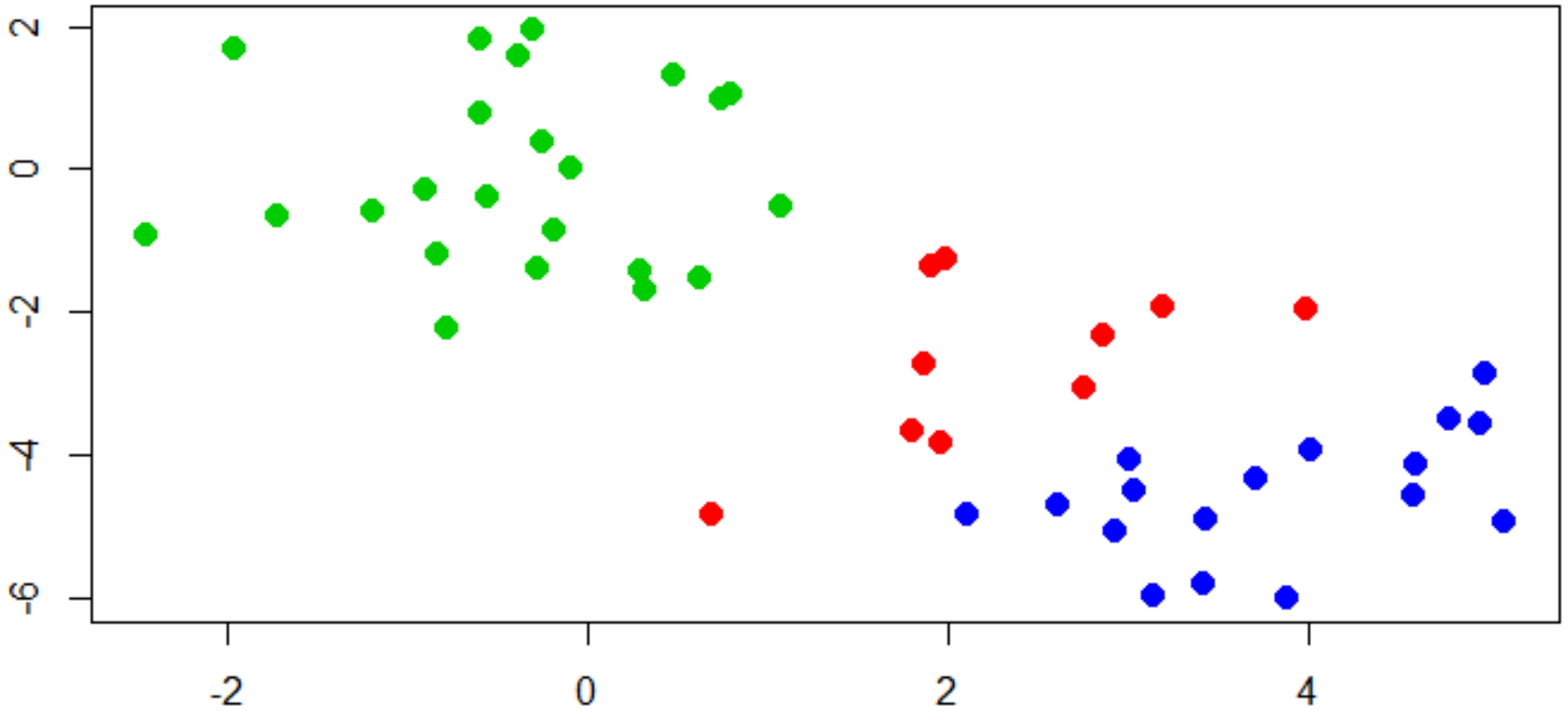
```
K-means clustering with 3 clusters of sizes 10, 23, 17

Cluster means:
         [,1]        [,2]
1   2.3001545 -2.69622023
2  -0.3820397 -0.08740753
3   3.7789567 -4.56200798

Clustering vector:
 [1] 3 1 3 1 3 3 3 1 3 1 3 1 3 1 3 1 3 3 3 3 3 1 3 3 3
[26] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 2 1 2 2 2 2

Within cluster sum of squares by cluster:
[1] 19.56137 52.67700 25.74089
 (between_SS / total_SS =  79.3 %)
```

plot(x, col=(km.out$cluster+1), xlab="", ylab="", pch=20, cex=2)



set.seed(3)

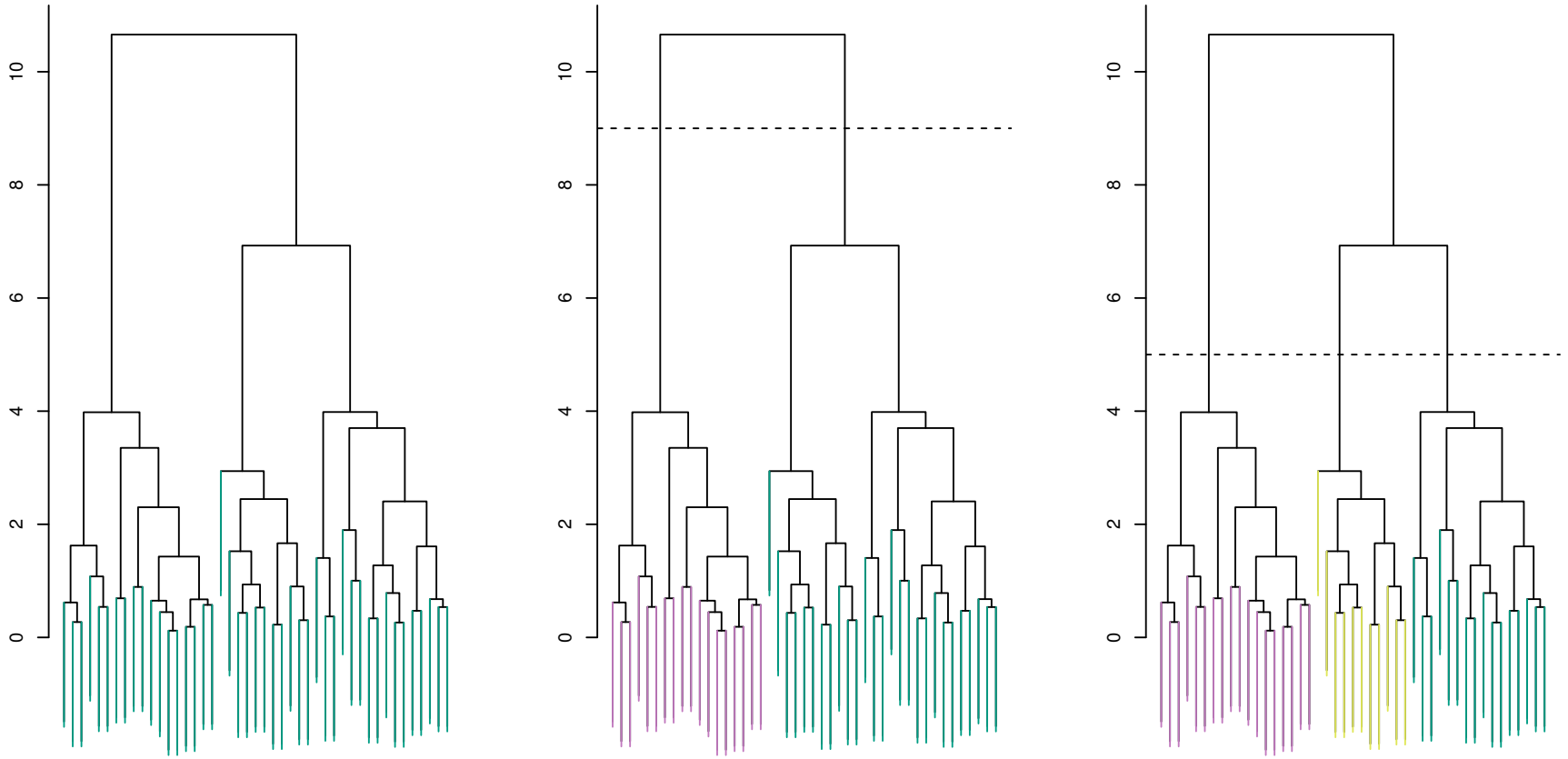
```
km.out=kmeans(x,3,nstart=1)
km.out$tot.withinss
```

104.33

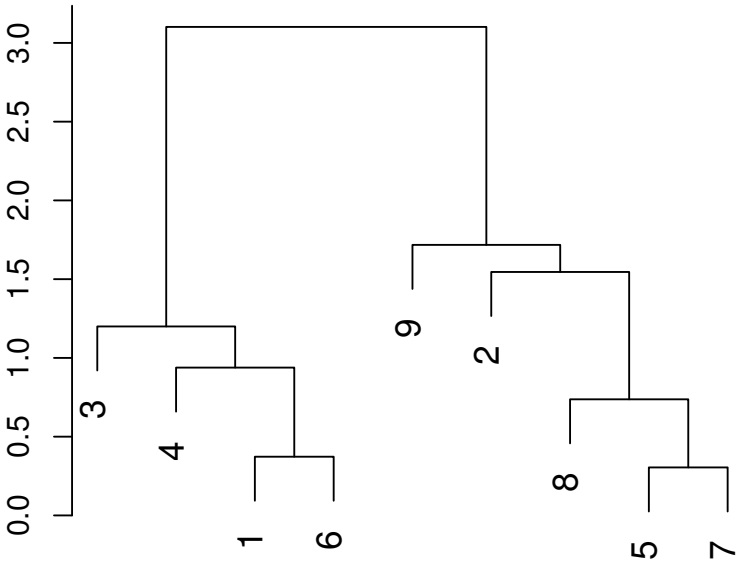
```
km.out=kmeans(x,3,nstart=20)
km.out$tot.withinss
```

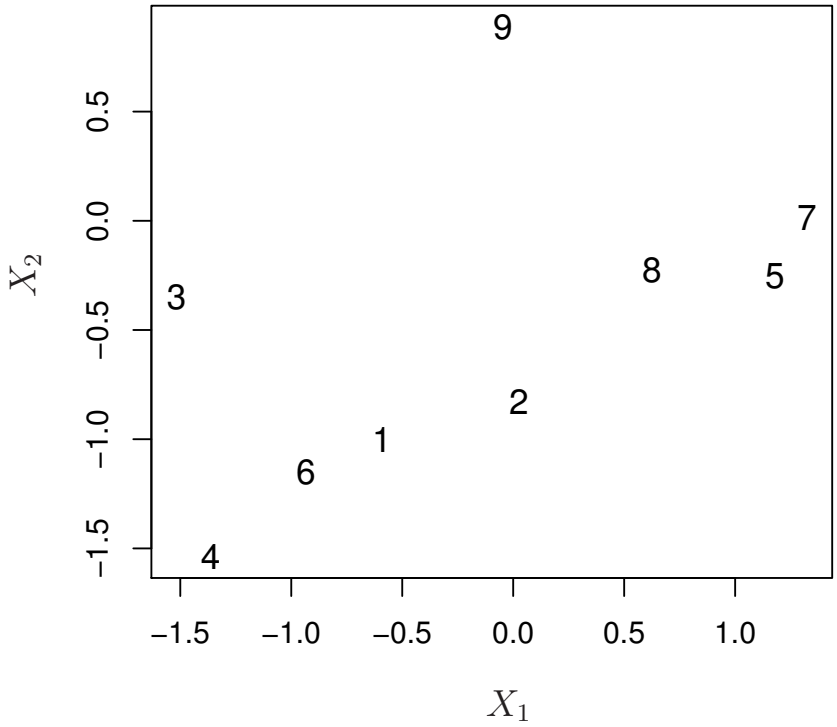
97.97

Hierarchical Clustering - Dendrogram



9 Observations: Euclidean Distance and Complete Linkage





Measure of Dissimilarity ($d(G, H)$)

Single Linkage or Nearest-Neighbor

$$\min_{i \in G, i' \in H} d_{ii'}$$

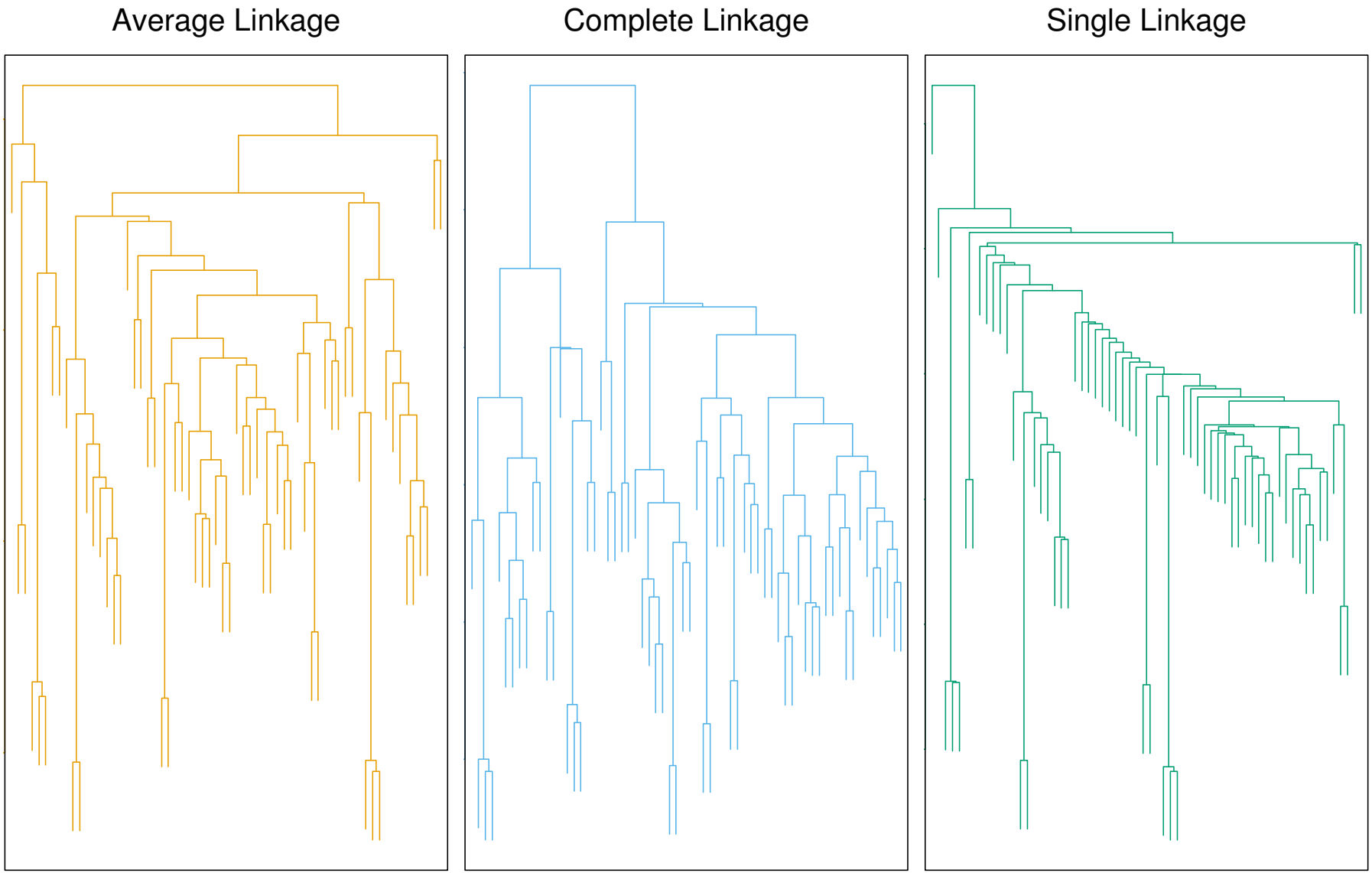
Complete Linkage or Furthest-Neighbor

$$\max_{i \in G, i' \in H} d_{ii'}$$

Group Average

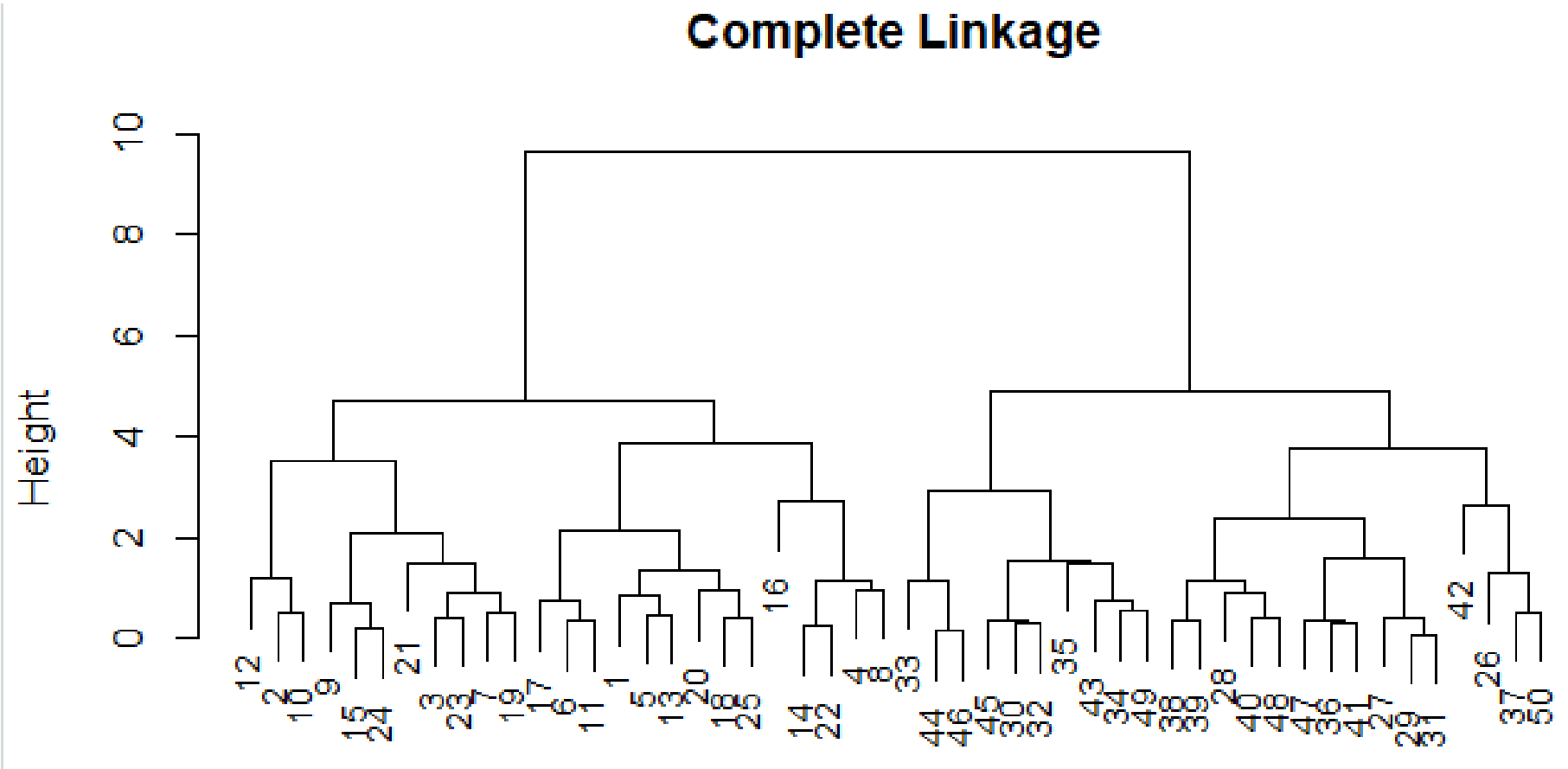
$$\frac{1}{N_G N_H} \sum_{i \in G} \sum_{i' \in H} d_{ii'}$$

Average, Complete, and Single Linkage



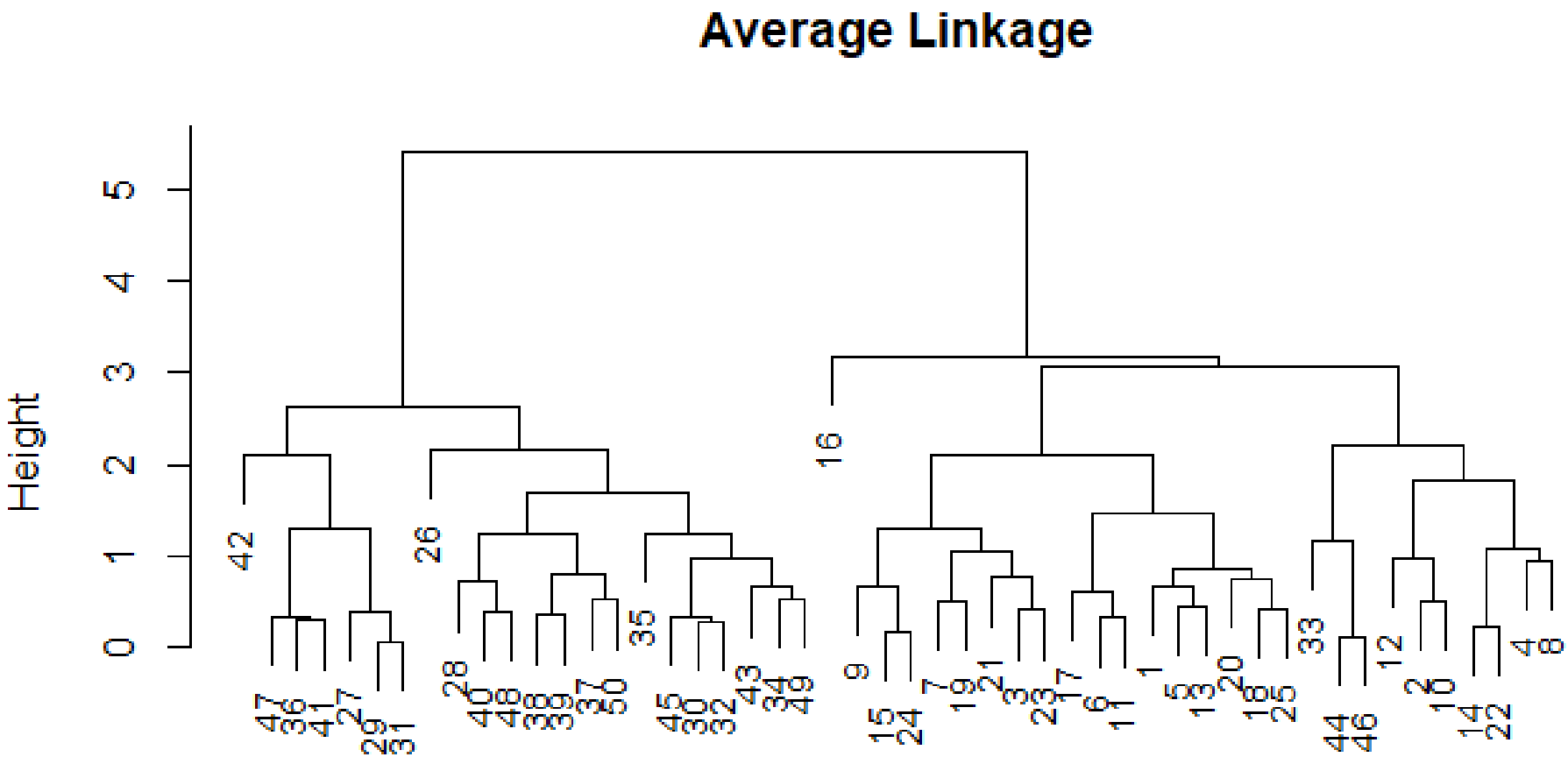
hc.complete=hclust(dist(x), method="complete")

plot(hc.complete,main="Complete Linkage", xlab="", sub="", cex=.9)



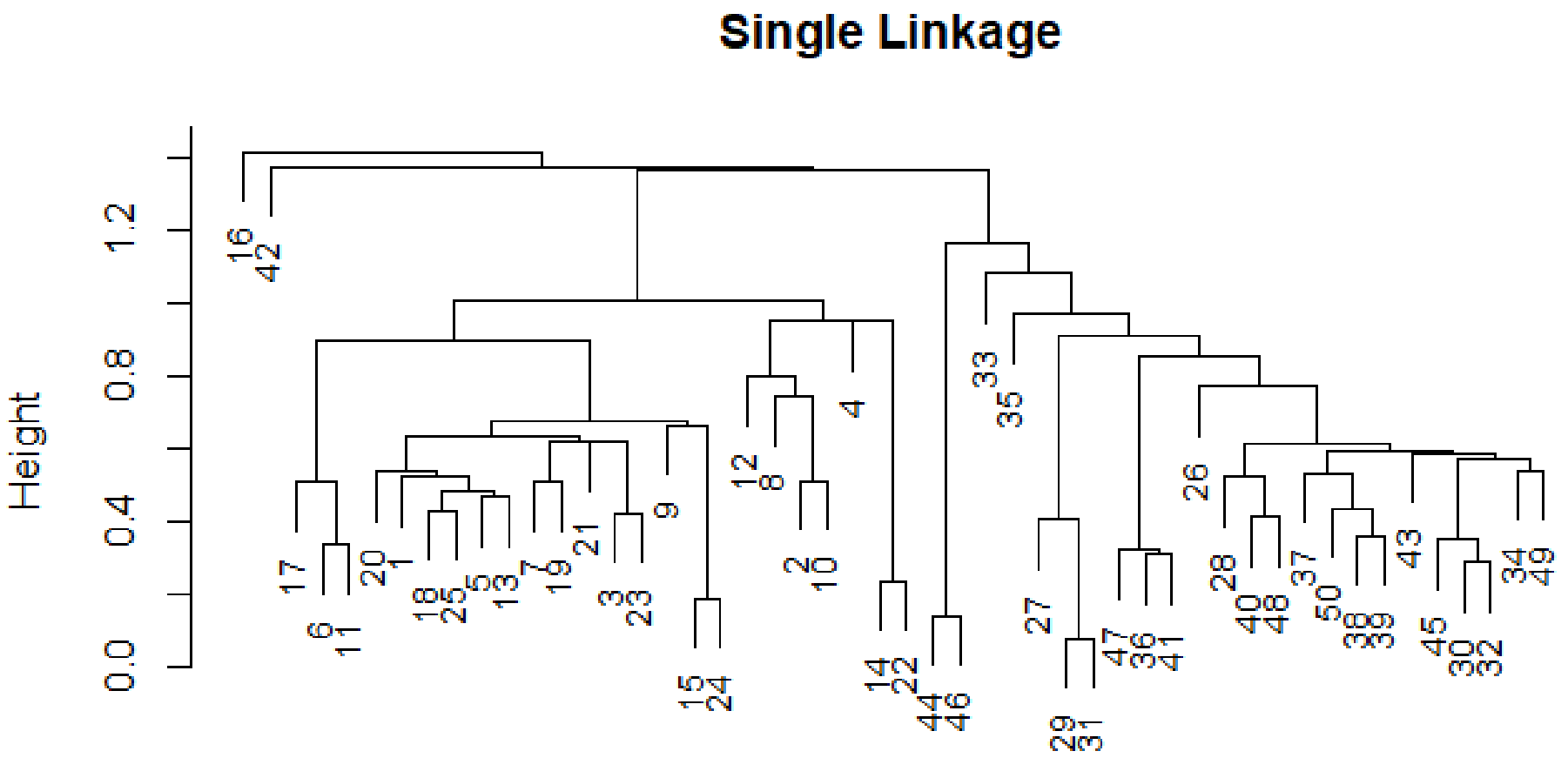
hc.average=hclust(dist(x), method="average")

plot(hc.average, main="Average Linkage", xlab="", sub="", cex=.9)



hc.single=hclust(dist(x), method="single")

plot(hc.single, main="Single Linkage", xlab="", sub="", cex=.9)



cutree(hc.complete, 2)

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
[26] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

cutree(hc.average, 2)

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
[26] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

cutree(hc.single, 2)

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
[26] 2 2 2 2 2 2 2 1 2 2 2 2 2 2 2 2 2 2 1 2 1 2 2 2 2 2
```

cutree(hc.single, 4)

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1
[26] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 4 3 3 3 3 3 3 3 3 3 3
```

library(ISLR)

```
nci.labs=NCI60$labs
nci.data=NCI60$data
dim(nci.data)
```

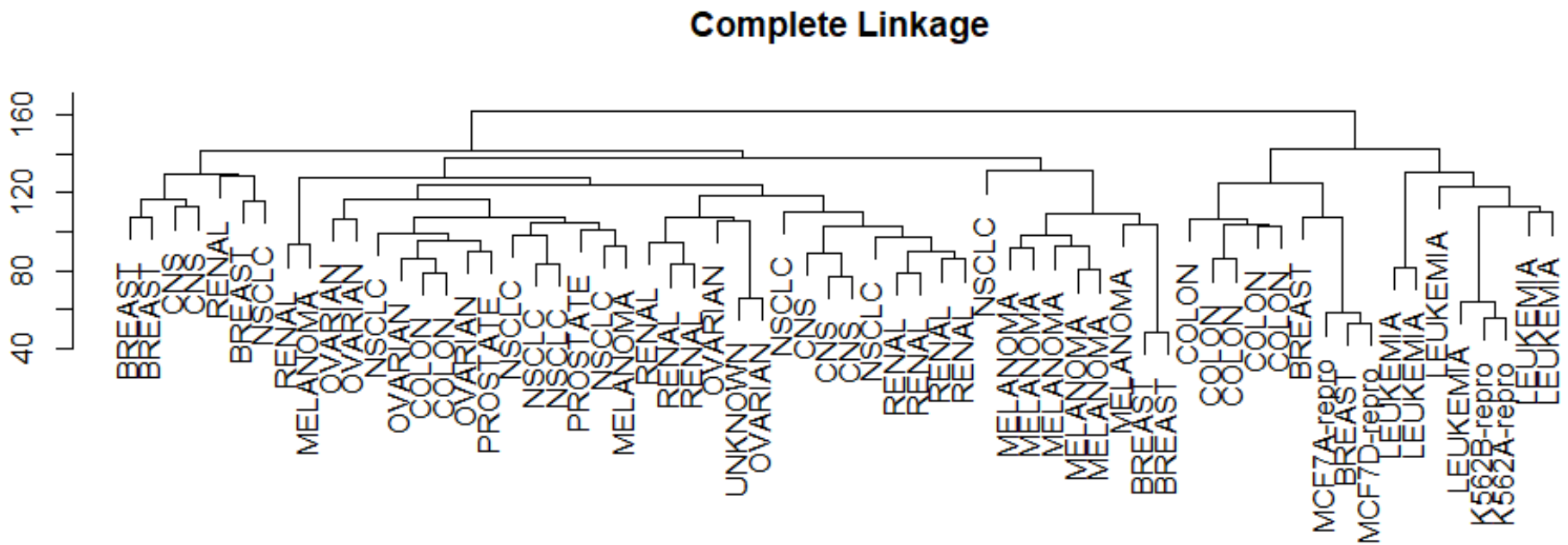
64 6830

```
table(nci.labs)
```

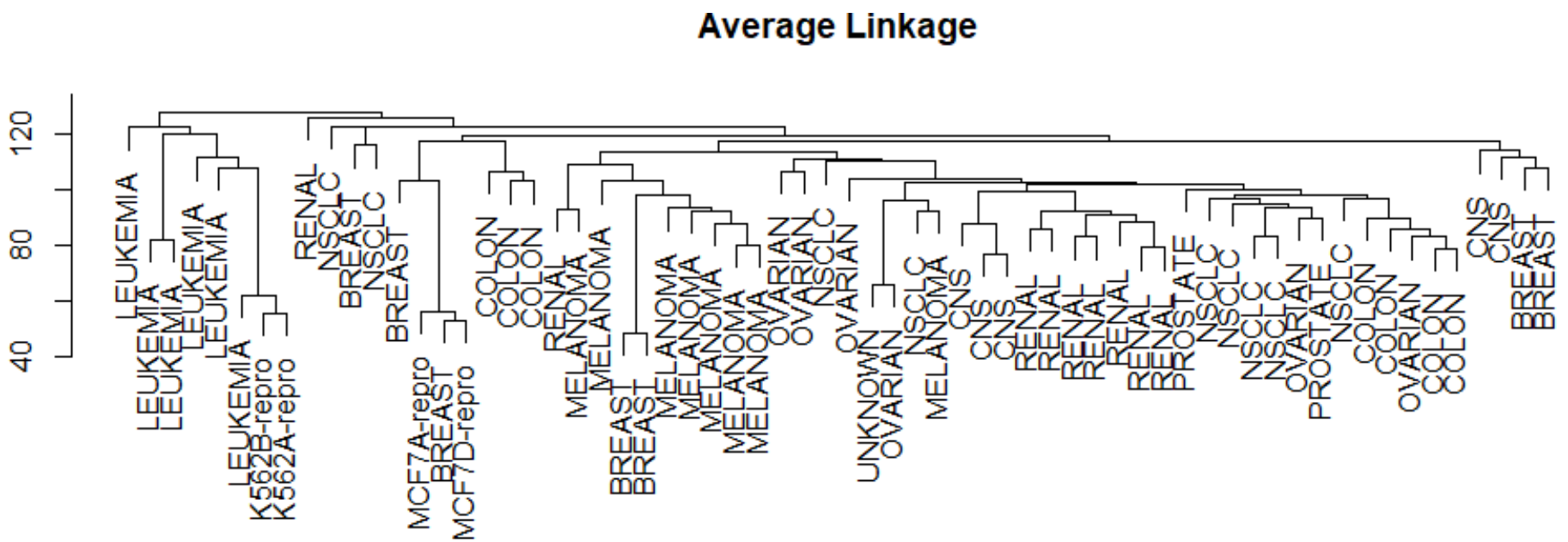
```
     BREAST         CNS       COLON K562A-repro K562B-repro
          7           5           7           1           1
    LEUKEMIA MCF7A-repro MCF7D-repro    MELANOMA       NSCLC
          6           1           1           8           9
     OVARIAN    PROSTATE       RENAL     UNKNOWN
          6           2           9           1
```

sd.data=scale(nci.data); data.dist=dist(sd.data)

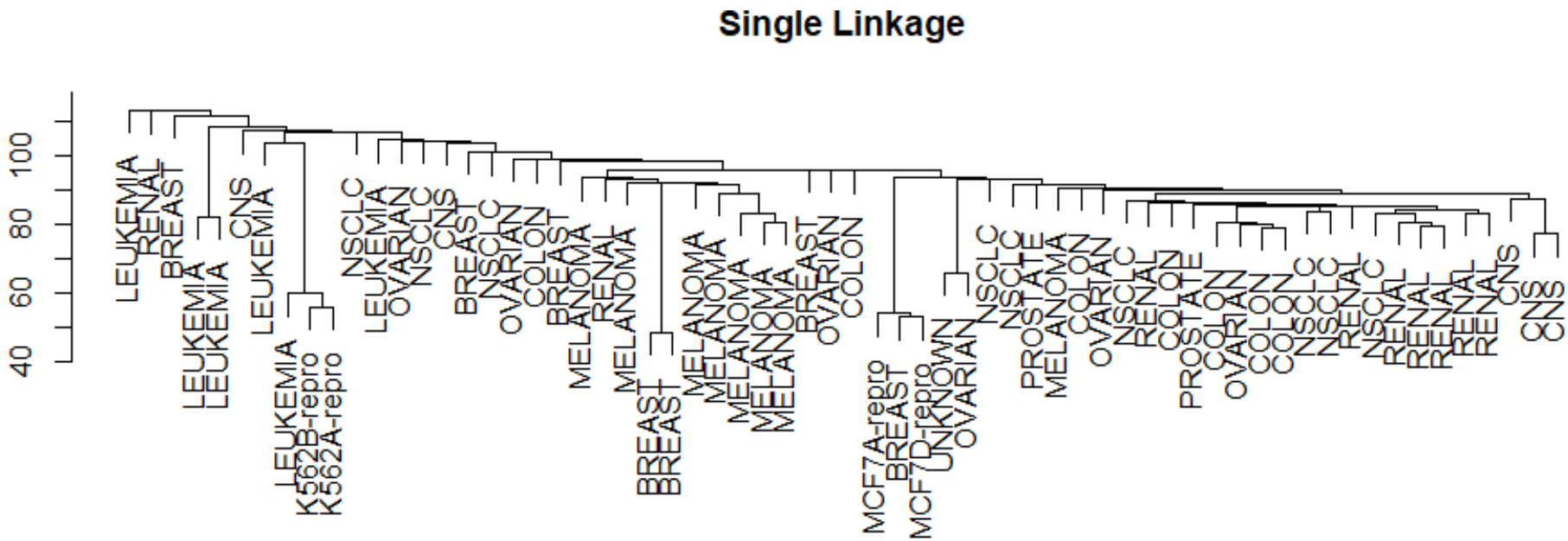
plot(hclust(data.dist), labels=nci.labs, main="Complete Linkage", xlab="", sub="",ylab="")



```
plot(hclust(data.dist, method="average"),
labels=nci.labs, main="Average Linkage", xlab="",
sub="",ylab="")
```



```
plot(hclust(data.dist, method="single"), labels=nci.labs, main="Single Linkage", xlab="", sub="",ylab="")
```



hc.out=hclust(dist(sd.data))

```
hc.out=hclust(dist(sd.data))
hc.clusters=cutree(hc.out,4)
table(hc.clusters,nci.labs)
```

```
            nci.labs
hc.clusters BREAST CNS COLON K562A-repro K562B-repro LEUKEMIA MCF7A-repro
          1      2   3     2           0           0        0           0
          2      3   2     0           0           0        0           0
          3      0   0     0           1           1        6           0
          4      2   0     5           0           0        0           1
            nci.labs
hc.clusters MCF7D-repro MELANOMA NSCLC OVARIAN PROSTATE RENAL UNKNOWN
          1           0        8     8       6         2     8       1
          2           0        0     1       0         0     1       0
          3           0        0     0       0         0     0       0
          4           1        0     0       0         0     0       0
```

set.seed(2)

```
km.out=kmeans(sd.data, 4, nstart=20)
km.clusters=km.out$cluster
table(km.clusters,hc.clusters)
```

	hc.clusters			
km.clusters	1	2	3	4
1	11	0	0	9
2	0	0	8	0
3	9	0	0	0
4	20	7	0	0