STAT406- Methods of Statistical Learning Lecture 21

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Unsupervised learning

- Unsupervised $\neq$ Supervised
- High-“density” regions (w/o model)
- Agglomerative / hierarchical methods
- High-“density” regions (with a model)
  - EM-algorithm
- Dimension reduction (PCA, MDS, etc.)

Clustering - Problem

- Data: p features / variables per "unit"

$$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{pmatrix}$$

- $\mathbf{X}_1, \ldots, \mathbf{X}_n$

Clustering

- Goal: find **regions** where $\mathbf{X}_i$'s are "clustered"
- Goal: find **regions** where $P(\mathbf{X})$ is relatively high
- These **regions** are sometimes modeled

Clustering

- Lower dimensional subspaces (linear manifolds)

  Principal Components

- Convex regions with high $P(\mathbf{X})$

  K-means / K-medoids – Hierarchical methods

Clustering

- Intrinsically different from **classification**

- There is no clear performance measure to evaluate “success”

- Hence the name: “unsupervised learning”

Clustering

Example 1 – 9 Breweries - 26 attributes

```
> a
   [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [...]
V1 3.51 3.41 3.20 2.73 2.35 3.03 2.21 3.91 3.07 [...]
V2 4.43 4.05 3.66 5.25 3.88 4.23 3.27 2.71 4.08 [...]
V3 4.76 3.42 4.22 2.44 4.18 2.47 3.67 4.59 4.74 [...]
V4 3.68 3.78 3.07 2.75 2.78 3.12 2.49 3.91 3.34 [...]
V5 4.77 1.04 3.86 5.28 3.86 4.24 3.40 4.23 4.23 [...]
[...]
   [,15] [,16] [,17] [,18] [,19] [,20] [,21] [,22] [...]
V1  3.07  3.45  2.53  3.12  2.93  2.24  2.41  3.32 [...]
V2  3.82  4.29  4.71  3.58  3.27  3.11  3.14  3.74 [...]
V3  4.17  4.44  4.53  4.10  4.13  4.12  3.43  4.32 [...]
V4  3.21  3.74  2.83  3.14  2.80  2.39  2.40  3.32 [...]
V5  3.94  4.47  4.83  3.82  3.46  3.39  3.22  4.01 [...]
[...]
```

Clustering

$$\mathbf{X}_1, \ \mathbf{X}_2, \ \ldots \ \mathbf{X}_9 \ \in \ \mathbb{R}^{26}$$

Do they appear grouped / clustered?

UN Votes

- From `http://hdl.handle.net/1902.1/12379`
- UN, founded 1946, 193 members
- “important” votes (U.S. State Department)
- Votes: Yes (1), Abstain (2), No (3), Absent (8), Not a Member (9)
- 368 important votes, 77 countries voted $\geq$ 95% of these

UN Votes

- Do voting patterns reflect political alignments?
- Do countries vote along known political blocks?
- Data: $\mathbf{X}_i$: votes for country i

$$\mathbf{X}_i \in \mathbb{R}^{368} \, , \quad i = 1, \ldots, 77 \text{ (countries)}$$

What groups are there?

Cancer example

- From [HTF09], details in script
- Gene expression for 64 samples
- There are 6830 genes
- $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_{64} \in \mathbb{R}^{6830}$
- We know tissue type for ea. sample
- Really: "**feature selection**"

K-means / K-medoids

- Look for convex sets of relative high density
- The number of sets **K** is specified *a priori* (but we'll come back to this)
- Since “high density” is related to “closeness”

$$\min \sum_{r=1}^{\mathbf{K}} \sum_{i,j \in \mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

minimize over all partitions $\mathcal{C}_1, \ldots, \mathcal{C}_K$

K-means / K-medoids

Note that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) = \sum_{r=1}^{\mathbf{K}}\sum_{i\in\mathcal{C}_r}\sum_{j=1}^{n} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

$$= \sum_{r=1}^{\mathbf{K}}\sum_{i\in\mathcal{C}_r}\left[\sum_{j\in\mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) + \sum_{j\notin\mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right)\right]$$

$$\sum_{r=1}^{\mathbf{K}}\sum_{i,j\in\mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) + \sum_{r=1}^{\mathbf{K}}\sum_{i\in\mathcal{C}_r}\sum_{j\notin\mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

$$T = \qquad W \qquad + \qquad B$$

K-means / K-medoids

When $d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) = \left\|\mathbf{X}_i - \mathbf{X}_j\right\|^2$

$$W = \sum_{r=1}^{K} \sum_{i,j \in \mathcal{C}_r} \left\|\mathbf{X}_i - \mathbf{X}_j\right\|^2 = \sum_{r=1}^{K} \sum_{i \in \mathcal{C}_r} \left\|\mathbf{X}_i - \bar{\mathbf{X}}_r\right\|^2$$

- Given $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_K$, assign $\mathbf{X}_i$ to the cluster $\mathcal{C}_j$ with closest mean

$$\mathbf{X}_i \quad \leftarrow \quad \arg \min_{1 \le \mathbf{j} \le K} \left\|\mathbf{X}_i - \bar{\mathbf{X}}_{\mathbf{j}}\right\|^2$$

K-means / K-medoids

- Note that

$$\bar{\mathbf{X}}_r \; = \; \hat{\mu}_r \; = \; \arg\min_{\boldsymbol{\mu}} \sum_{i \in \mathcal{C}_r} \| \mathbf{X}_i - \boldsymbol{\mu} \|^2$$

- Given $\hat{\mu}_1, \ldots, \hat{\mu}_K$

$$\min_{\mathcal{C}_{\mathbf{1}}, \ldots, \mathcal{C}_{\mathbf{k}}} \sum_{r=1}^{k} \sum_{i \in \mathcal{C}_{\mathbf{r}}} \| \mathbf{x}_i - \hat{\mu}_r \|^2$$

is attained with

$$\mathbf{X}_i \quad \leftarrow \quad \arg \min_{1 \le j \le K} \left\| \mathbf{X}_i - \hat{\mu}_j \right\|^2$$

K-means / K-medoids

- And, given $\mathcal{C}_1, \ldots, \mathcal{C}_K$

$$\min_{\hat{\mu}_1, \ldots, \hat{\mu}_K} \sum_{r=1}^{k} \sum_{i \in \mathcal{C}_r} \| \mathbf{x}_i - \hat{\mu}_r \|^2$$

is attained with

$$\hat{\mu}_r \quad \leftarrow \quad \bar{\mathbf{X}}_r \; = \; \frac{1}{n_r} \sum_{i \in \mathcal{C}_r} \mathbf{x}_i$$

This suggests a simple iterative (and greedy) algorithm.

K-means / K-medoids

Remarks

- Algorithm is greedy
- Answer depends on the initial configuration
- It needs to be started from **many initial configurations**

Cancer data

```
> set.seed(31)
> nci.km <- kmeans(nci, centers=8)
> table(nci.km$cluster)

 1  2  3  4  5  6  7  8 
 8  6  6 14  3  8  4 15 

> set.seed(311)
> nci.km <- kmeans(nci, centers=8)
> table(nci.km$cluster)

 1  2  3  4  5  6  7  8 
 4 12  6  9  4  8 19  2 
```

K-means / K-medoids

Need **more** starting points...

```
> set.seed(31)
> nci.km <- kmeans(nci, centers=8, iter.max = 5000,
  nstart=1000)
> table(nci.km$cluster)

 1  2  3  4  5  6  7  8 
 3  8  5 14  6 15  9  4 

> set.seed(311)
> nci.km <- kmeans(nci, centers=8, iter.max = 5000,
  nstart=1000)
> table(nci.km$cluster)

 1  2  3  4  5  6  7  8 
 4  5  8  9 14  3 15  6 
```

These clusters are the same

K-means / K-medoids

Tissue	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
LEUKEMIA	1		**5**					
BREAST		2			1		2	2
RENAL		1			**8**			
COLON				1		**6**		
PROSTATE				2				
MELANOMA					1		**7**	
OVARIAN				**5**	1			
NSCLC				**6**	3			
OTHER	2	**5**			1			2

UN Votes example

- Not all countries voted each time

```
> dim(X)
[1] 368  77
> sum( complete.cases(X) )
[1] 145
```

- Only use resolutions with full votes

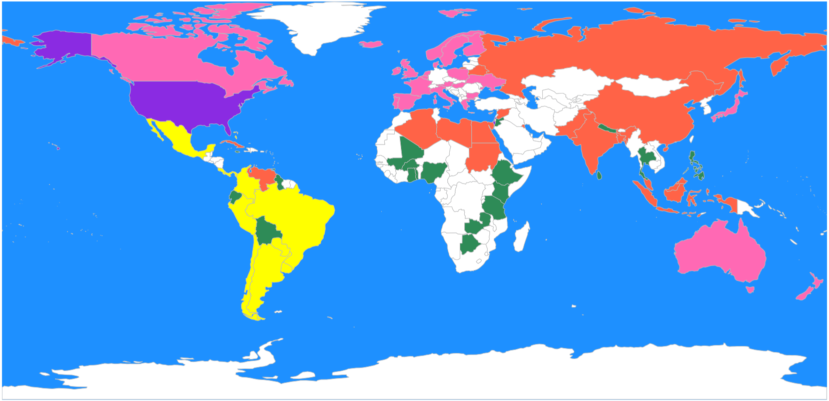
```
X2 <- X[complete.cases(X),]
```

- Use `kmeans` in `R`

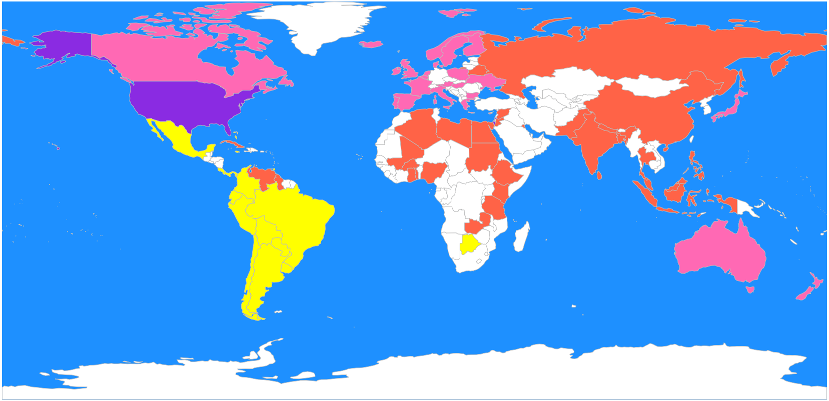
UN Votes example

```
> set.seed(123)
> b <- kmeans(t(X2), centers=5,
                     iter.max=20, nstart=1)
> table(b$cluster)

 1  2  3  4  5 
18  2  7 19 31 
> b <- kmeans(t(X2), centers=5,
                     iter.max=20, nstart=1)
> table(b$cluster)

 1  2  3  4  5 
27 12 13  7 18 
```

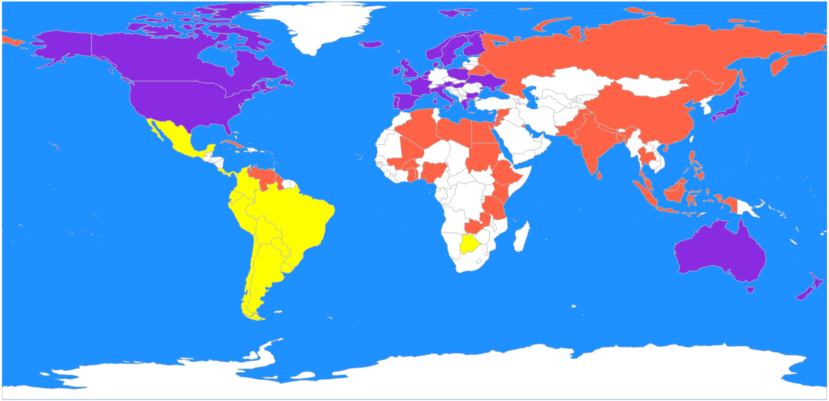
UN Votes example - K=5



UN Votes example - K=4



UN Votes example - K=3



K-means++

- A cleverly chosen set of initial centres
- K-means++
  - Pick a centre $\mathbf{c}_1$ at random (from data)
  - Then `for j in 2:k`
    - Compute weights

      $$w_i = \min \left(d^2(\mathbf{x}_i, \mathbf{c}_1), \ldots, d^2(\mathbf{x}_i, \mathbf{c}_{j-1}) \right) \, , \quad i = 1, \ldots, n$$

    - Pick next centre $\mathbf{c}_j$ from data with prob $\propto d_i$
- Implemented in `flexclust::kcca`

Choosing K

For each cluster $\mathcal{C}_r$, let

$$W\left(\mathcal{C}_r\right) = \sum_{j,i \in \mathcal{C}_r} d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) \qquad r = 1, \ldots, \mathbf{K}$$

and

$$W_{\mathbf{K}} = \sum_{j=1}^{\mathbf{K}} W\left(\mathcal{C}_r\right)$$

Choosing K

- Note that selecting **K** to minimize $W_{\mathbf{K}}$ does not generally work
- $W_{\mathbf{K}}$ typically decreases with **K**
- A simple example follows

Selecting the number K of clusters

For each cluster $\mathcal{C}_r$, let

$$W(\mathcal{C}_r) = \sum_{j,i \in \mathcal{C}_r} d\left(\mathbf{X}_i, \mathbf{X}_j\right) \qquad r = 1, \ldots, \mathbf{K}$$

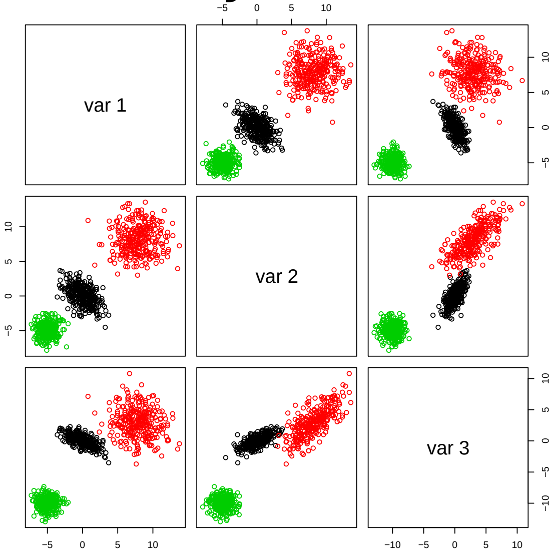
and

$$W_{\mathbf{K}} = \sum_{j=1}^{\mathbf{K}} W(\mathcal{C}_r)$$

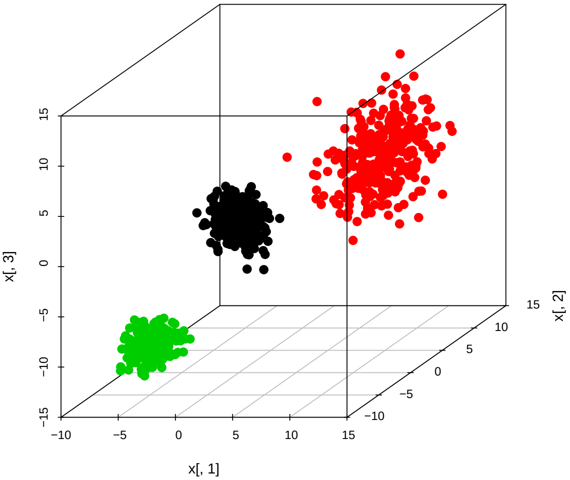
Selecting the number K of clusters

- Note that selecting **K** to minimize $W_{\mathbf{K}}$ does not generally work
- $W_{\mathbf{K}}$ typically decreases with **K**
- A simple example follows

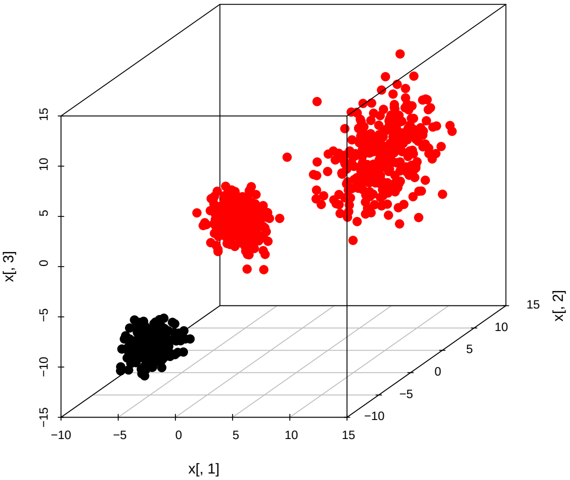
Pairs plot - Easy case



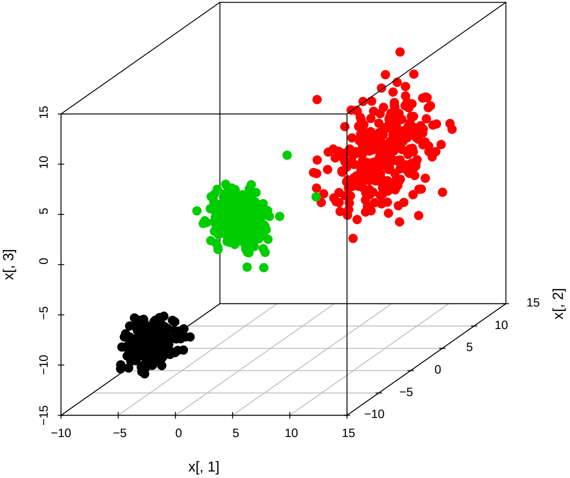
Pairs plot - Easy case



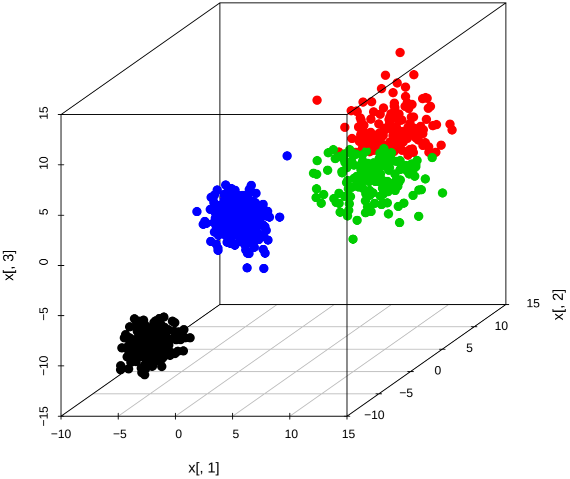
Pairs plot - K-means - K = 2



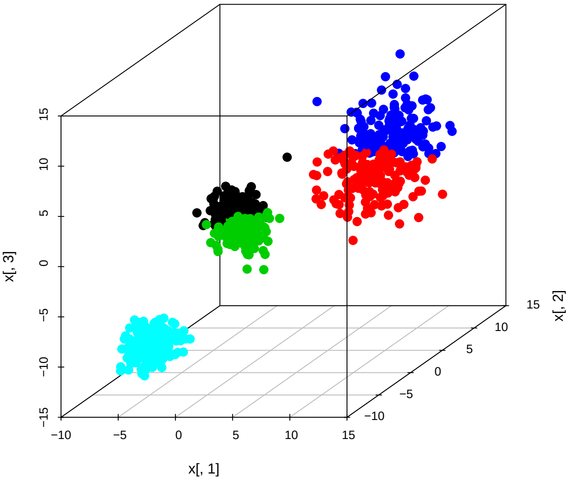
Pairs plot - K-means - K = 3



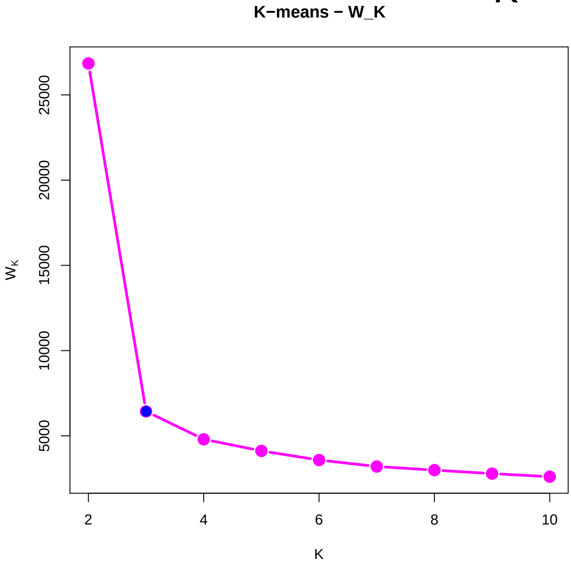
Pairs plot - K-means - K = 4



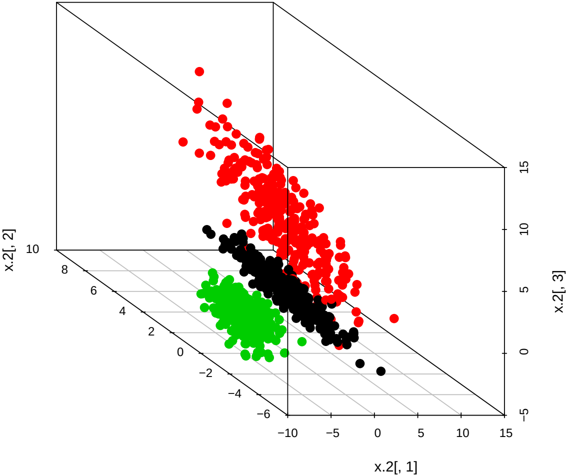
Pairs plot - K-means - K = 5



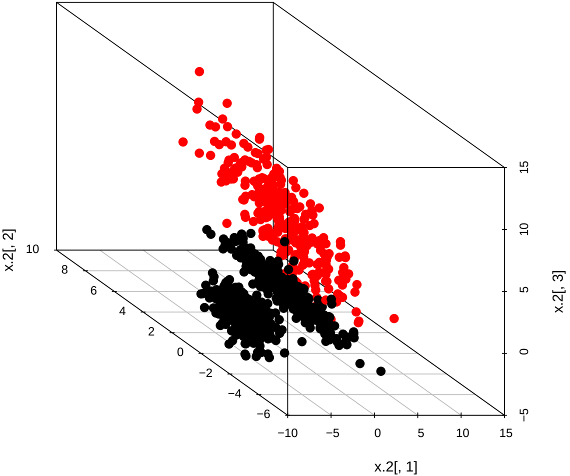
Pairs plot - K-means - W_K



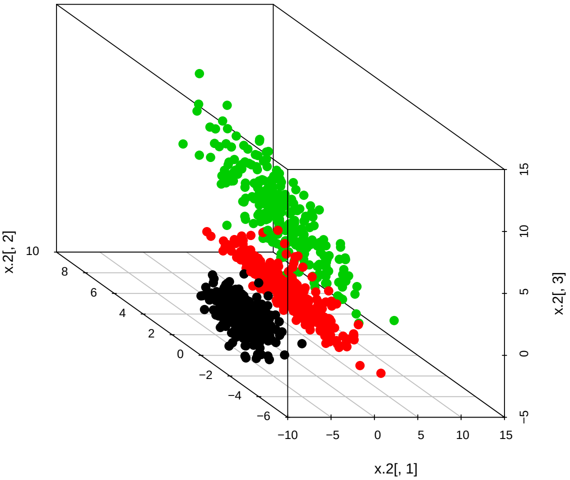
Pairs plot - K-means



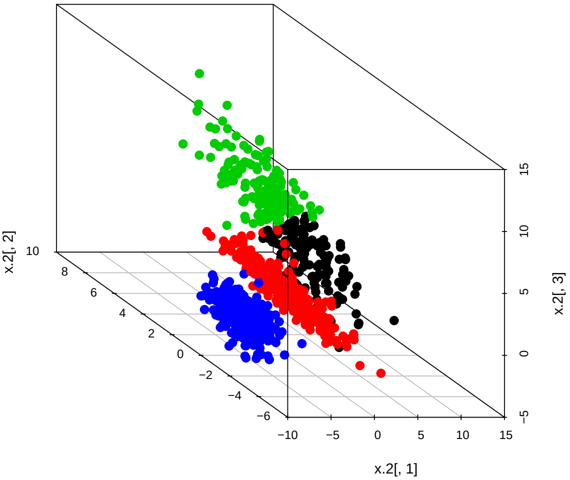
Pairs plot - K-means - K = 2



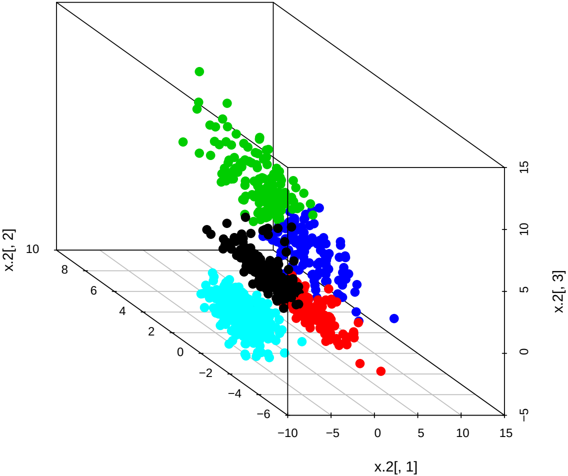
Pairs plot - K-means - K = 3



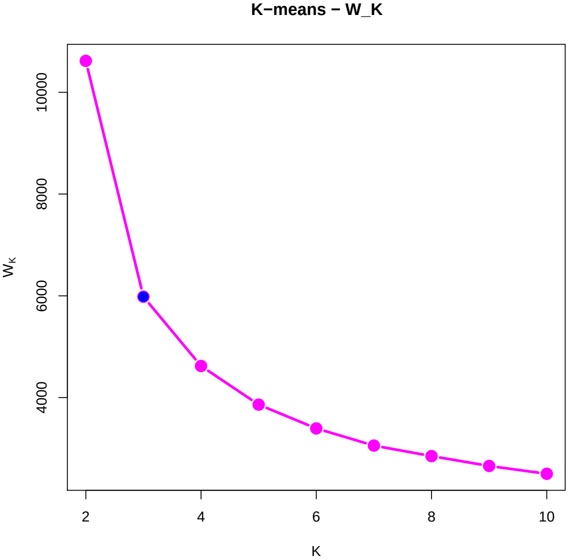
Pairs plot - K-means - K = 4



Pairs plot - K-means - K = 5



Pairs plot - K-means - W_K



GAP Statistic

GAP Statistic (Tibshirani, Walther and Hastie, 2001)

Consider

$$G(\mathbf{K}) = E[\log(W_{\mathbf{K}})] - \log(W_{\mathbf{K}})$$

where $E[\log(W_{\mathbf{K}})]$ is the expected value under a certain reference distribution

Clest algorithm

Clest algorithm

Idea - select the value of **K** that produces classes that are best predicted by your favourite classification method.

Dudoit, Fridlyand, 2002, A prediction-based resapmling method for estimating the number of clusters in a dataset, Genome Biology **3(7)** : research0036.1 - 0036.21

Other approaches to select **K**

Dudoit, Fridlyand, 2003, Bagging to improve the accuracy of a clustering procedure, Bioinformatics, **19**, 1090-1099

K-means / K-medoids

Note that in K-means

- We used $d^2\left(\mathbf{X}_i, \mathbf{X}_j\right) = \left\|\mathbf{X}_i - \mathbf{X}_j\right\|^2$
- The cluster “centers” may not be actual observations
- Need to manipulate the “features” ($\mathbf{X}_i$)
- Can we use different distance measures?
- Can we work with the dissimilarities only?

K-means / K-medoids

A slightly different algorithm is

- Given $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_K$, for each cluster $\mathcal{C}_r$ find

  $$j_r^* = \arg\min_{i \in \mathcal{C}_r} \sum_{j \in \mathcal{C}_r} d\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

  and let $m_r = \mathbf{X}_{j_r^*}$
- Given $m_1, m_2, \ldots, m_K$, assign $\mathbf{X}_i$ to the cluster $\mathcal{C}_j$ with closest centre:

$$\mathbf{X}_i \quad \leftarrow \quad \arg\min_{1 \le j \le K} d\left(\mathbf{X}_i, m_j\right)$$

K-means / K-medoids

1. Find K initial cluster centres
2. Given centres m_ℓ, assign points to the cluster $\mathcal{C}_j$ with closest centre:

$$\mathbf{X}_i \quad \leftarrow \quad \arg \min_{1 \le j \le K} d\left(\mathbf{X}_i, m_j\right)$$

3. Explore all possible swaps between centres and non-centres.
4. If there's improvement, go to step 2

K-means / K-medoids

Note that now

- We can use any distance – robustness?
- The cluster representatives / prototypes are actual observations
- We do not need the observations, only the dissimilarities

K-means / K-medoids

Beers - 9 beers with 26 attributes

```
> a <- read.table(’breweries.dat’, header=FALSE)
> a <- t(a)
> a.dis <- dist(a, method=’manhattan’)
>
> brew.pam <- pam(a.dis, k=3)
>
> brew.pam
Medoids:
     ID
[1,] "7" "V7"
[2,] "2" "V2"
[3,] "6" "V6"
Clustering vector:
V1 V2 V3 V4 V5 V6 V7 V8 V9
 1  2  3  1  2  3  1  3  2
```

Silhouette plot

- For each unit $\mathbf{X}_i \in \mathcal{C}_\ell$

$$a_i = \frac{1}{n_\ell} \sum_{\mathbf{X}_j \in \mathcal{C}_\ell} d\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

- Dissimilarity with other clusters

$$d\left(i, \mathcal{C}_r\right) = \frac{1}{n_r} \sum_{\mathbf{X}_j \in \mathcal{C}_r} d\left(\mathbf{X}_i, \mathbf{X}_j\right)$$

Silhouette plot

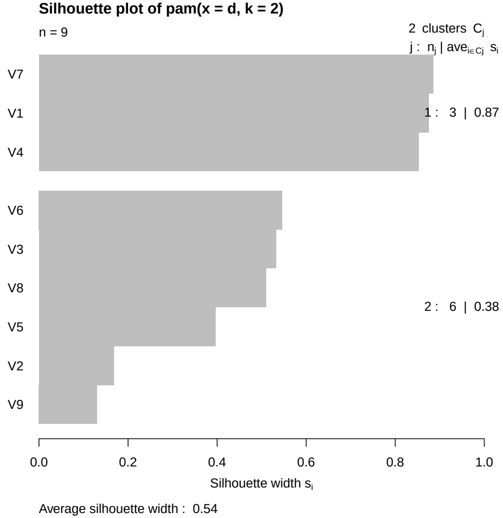
- Then, dissimilarity to closest cluster

$$b_i = \min_{r \neq \ell} d\left(i, \mathcal{C}_r\right)$$

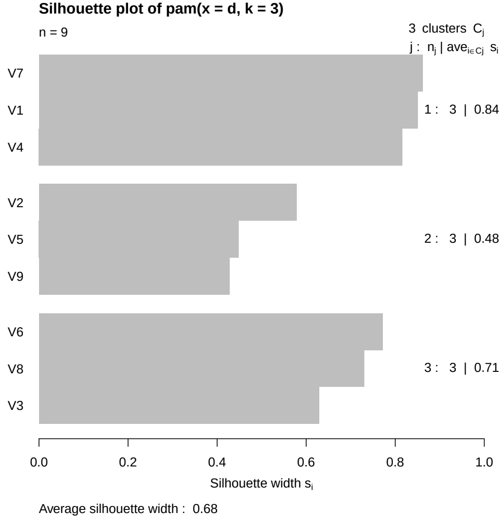
- Silhouette

$$s_i = \left(b_i - a_i\right) / \max\left(a_i, b_i\right)$$

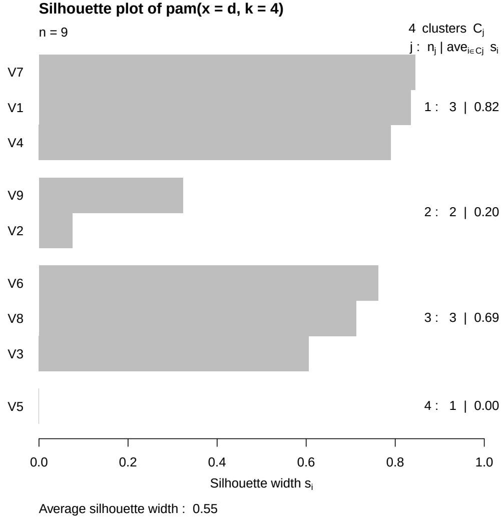
Breweries - K=2



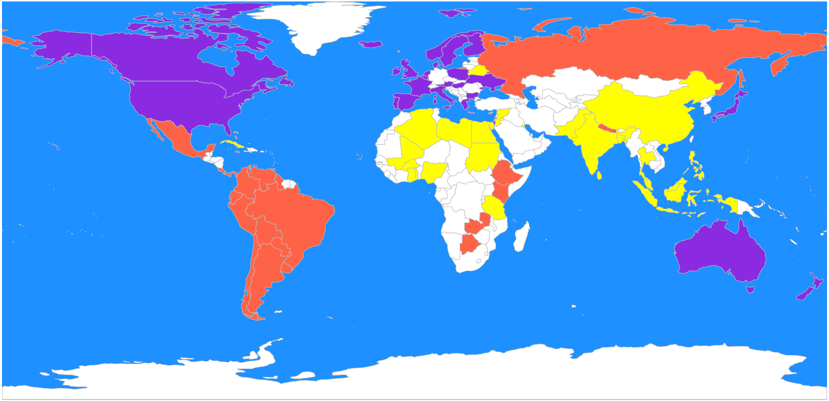
Breweries - K=3



Breweries - K=4



UN Votes PAM - K=3



UN Votes Kmeans - K=3