

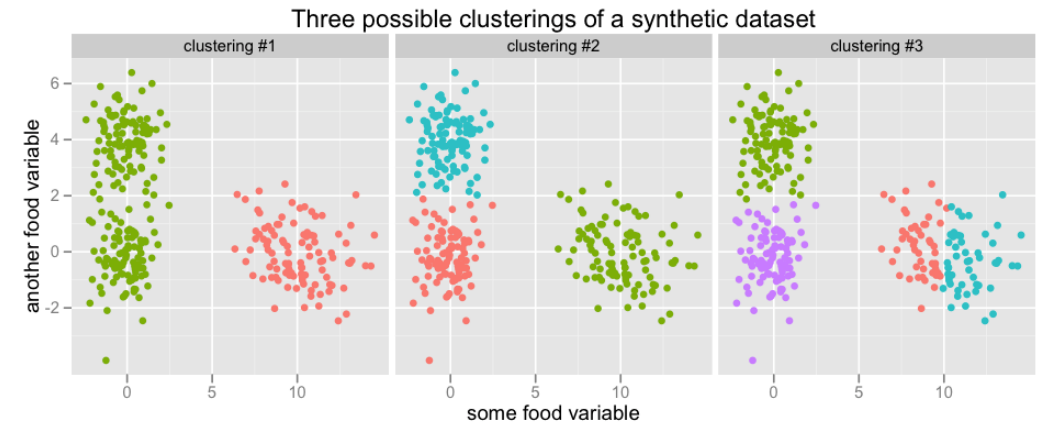
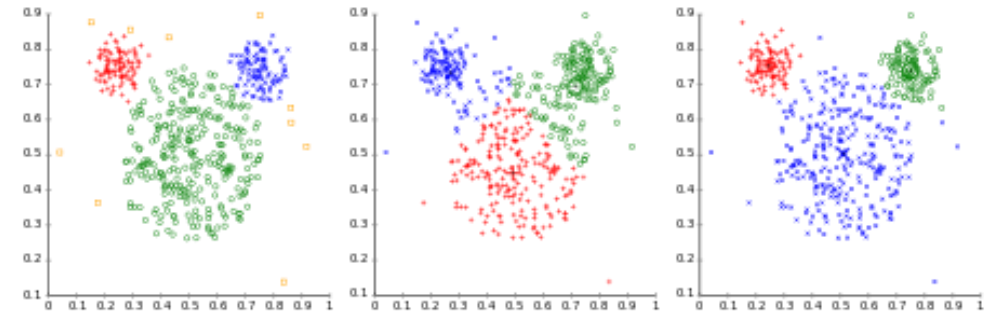
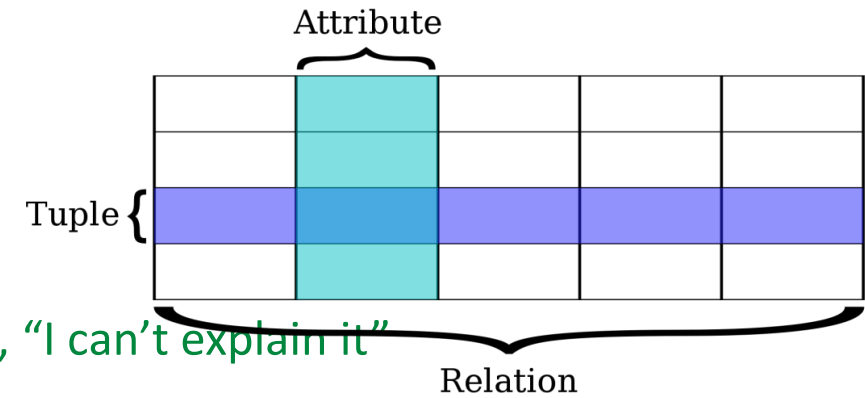
# Clustering

Praphul Chandra



# Clustering 101

- Motivation
  - Transaction data (Customer – Product matrix)
  - Test measurements from a fab plant for chips
  - Segmentation, Pre-processing, Multimodal distributions, “I can’t explain it”
- Clustering
  - Find elements (rows, tuples) which are similar.
  - Finding “areas” in space where data is concentrated
  - WYSIWYG : What You Select Is What You Get
- When are two elements / rows similar?
  - A measure of (dis)similarity.
  - Which dimensions (attributes) are relevant?
  - Normalization?
  - How many clusters?



# Similarity, Dissimilarity & Distance

Measures



# Distance in multiple dimensions

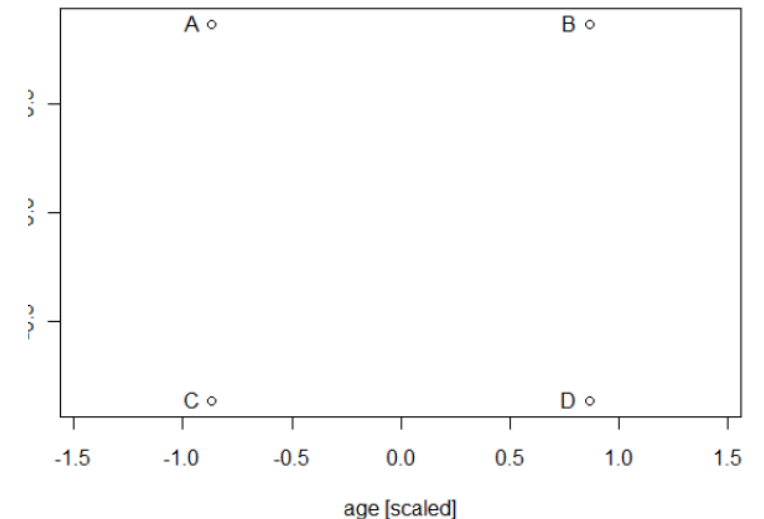
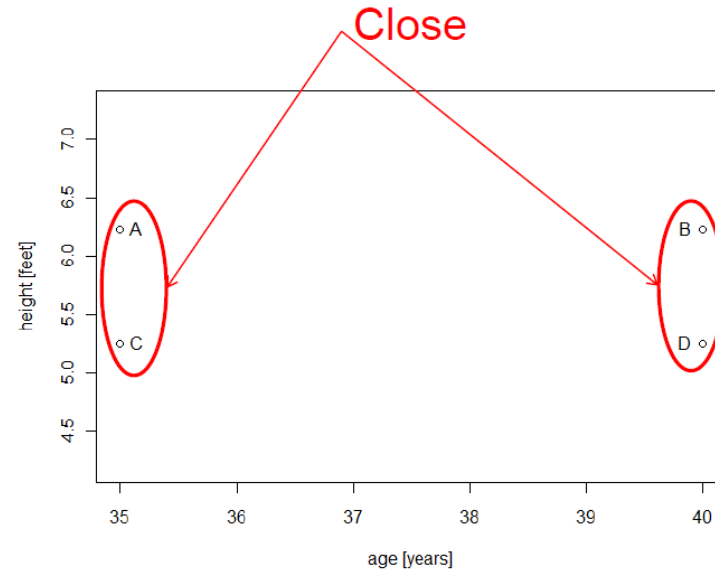
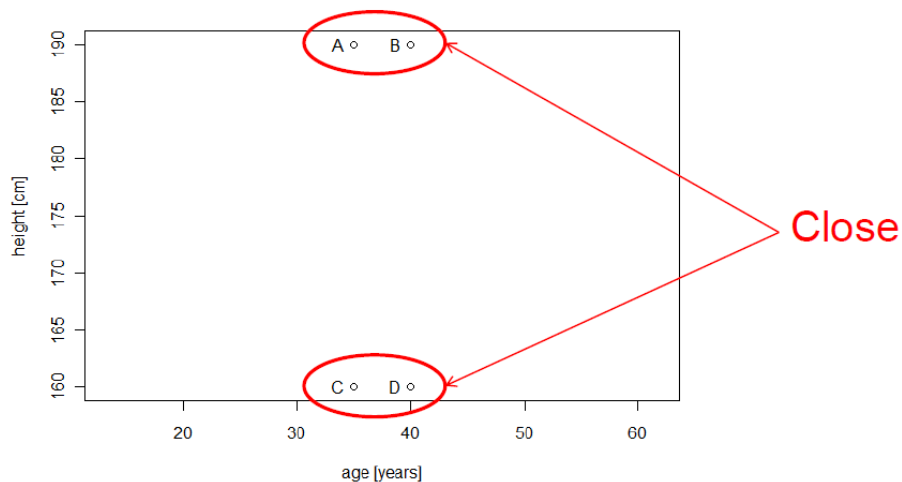
Euclidean distance:

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ip} - x_{jp})^2}$$

Person	Age [years]	Height [cm]
A	35	190
B	40	190
C	35	160
D	40	160

Person	Age [years]	Height [feet]
A	35	6.232
B	40	6.232
C	35	5.248
D	40	5.248

Person	Age [scaled]	Height [scaled]
A	-0.87	0.87
B	0.87	0.87
C	-0.87	-0.87
D	0.87	-0.87



# Distance in multiple dimensions : To Scale or Not

- Distance depends on scale
- If variables are not scaled
  - Variable with largest range has most weight

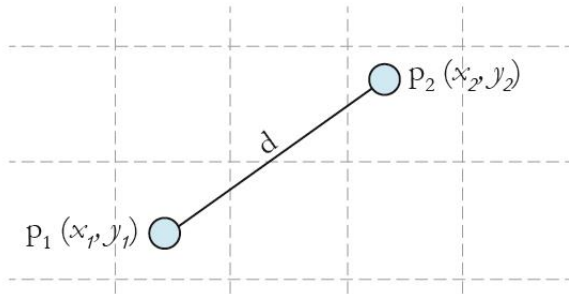
- If variables are scaled
  - Every variable gets equal weight
  - Similar alternative is re-weighting

$$d(i, j) = \sqrt{w_1(x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + \dots + w_p(x_{ip} - x_{jp})^2}$$

- Scale
  - If variables measure different units (kg, meter, sec,...)
  - If you explicitly want to have equal weight for each variable
  - Default
- Don't scale
  - if units are the same for all variables



# Measures of Dissimilarity : distance



Euclidean distance: L2 distance

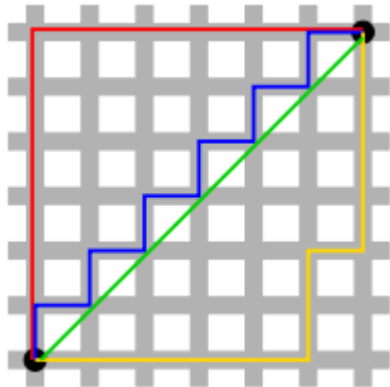
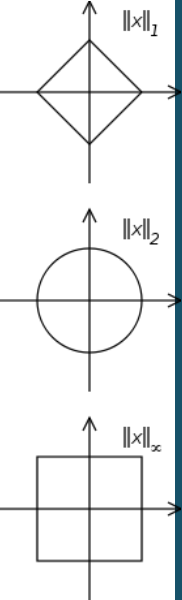
$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ip} - x_{jp})^2}$$

$$\|x_i\|_1 = \sum_p |x_j|$$

$$\|x_i\|_2 = \left( \sum_p |x_j|^2 \right)^{\frac{1}{2}}$$

$$\|x_i\|_z = \left( \sum_p |x_j|^z \right)^{\frac{1}{z}}$$

$$\|x_i\|_\infty = \max_p |x_j|$$



Manhattan distance: a.k.a. L1 distance a.k.a. Taxicab

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

Hamming distance = 3

A	1	0	1	1	0	0	1	0	0	1
			⊕				⊕		⊕	
B	1	0	0	1	0	0	0	0	1	1

Special cases of Minkowski distance:

$$d(i, j) = (|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \dots + |x_{ip} - x_{jp}|^q)^{\frac{1}{q}}$$

Maximum distance: a.k.a. L<sub>∞</sub> distance a.k.a. supremum (max. dist. in any dimension)

$$\begin{aligned} d(i, j) &= (|x_{i1} - x_{j1}|^\infty + |x_{i2} - x_{j2}|^\infty + \dots + |x_{ip} - x_{jp}|^\infty)^{\frac{1}{\infty}} = \\ &= \max_{k=1}^p |x_{ik} - x_{jk}| \end{aligned}$$



# Measures of Similarity : The Dot Product

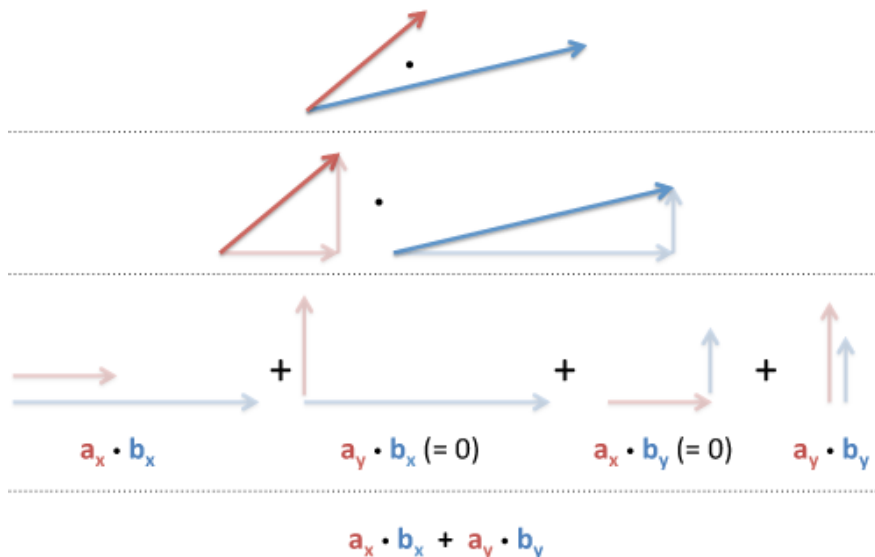
- Inner Product

- Element wise product of two vectors
- a.k.a. scalar product

$$\begin{pmatrix} 3 \\ -2 \\ 6 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \\ -5 \end{pmatrix} = 3 \times 2 + (-2) \times 3 + 6 \times (-5) = 6 - 6 - 30 = -30.$$

$$\mathbf{w} \in \mathbb{R}^p, \mathbf{x} \in \mathbb{R}^p$$

$$\mathbf{w}^T \mathbf{x} = \sum_{j=1}^p w_j x_j = \langle \mathbf{w}, \mathbf{x} \rangle$$



- Projection Product

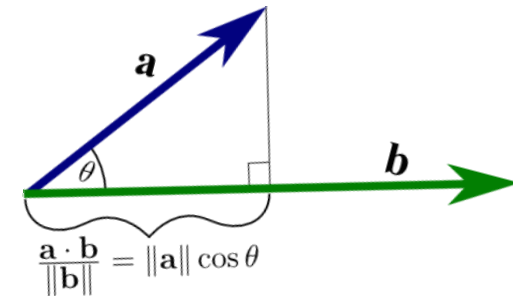
- Vector : Magnitude (Length) & Direction

$$\mathbf{w}^T \mathbf{x} = \|\mathbf{w}\| \|\mathbf{x}\| \cos \theta$$

$$\theta = 90 \Rightarrow \mathbf{w}^T \mathbf{x} = 0$$

$$\theta = 0 \Rightarrow \mathbf{w}^T \mathbf{x} = \|\mathbf{w}\| \|\mathbf{x}\|$$

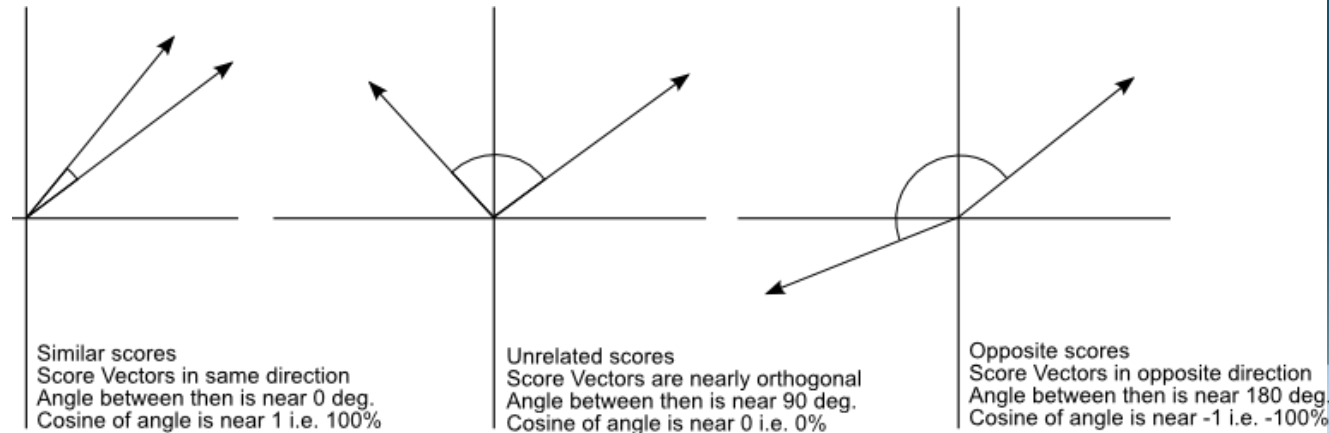
$$\mathbf{w}^T \mathbf{w} = \|\mathbf{w}\|^2$$



$$x_w = \|\mathbf{x}\| \cos \theta = \frac{\|\mathbf{x}\| \|\mathbf{w}\| \cos \theta}{\|\mathbf{w}\|} = \frac{\mathbf{x}^T \mathbf{w}}{\|\mathbf{w}\|} = \mathbf{x}^T \left( \frac{\mathbf{w}}{\|\mathbf{w}\|} \right) = \mathbf{x}^T \hat{\mathbf{w}}$$

# Measures of Similarity : Cosine Similarity

- Cosine of angle between two vectors
  - Distance between vectors captured by the cosine of the angle  $\times$  between them.
- a.k.a. normalized inner product
  - Denominator involves the lengths of the vectors
- Dot-products and Cosine Similarity
  - Relevant in information retrieval
  - Documents (query) as vectors of words
  - Two documents similar if they contain the same words
  - Does size of the document matter?
    - Yes: Dot Product
    - No: Cosine similarity



$$\text{similarity} = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$$





# Measures of dissimilarity : Categorical Variables

- Categorical Variables

- One hot encoding

- Hamming Distance

- Also useful for strings

$d(\text{"karolin"}, \text{"kathrin"}) = 3.$

$d(\text{"karolin"}, \text{"kerstin"}) = 3.$

$d(1011101, 1001001) = 2.$

$d(2173896, 2233796) = 3.$

- Coefficients

- SMC: Simple Matching Coefficient
- Jaccard coefficient
- Dice coefficient
- Custom Variants: if one of the states is more important or more valuable than the other.
- Distance = 1 - coefficient

a		a	a1	a2	a3
1	→	1	1	0	0
2		2	0	1	0
3		3	0	0	1

$p = 1000000000$

$q = 0000001001$

$M_{01} = 2$  (the number of attributes where p was 0 and q was 1)

$M_{10} = 1$  (the number of attributes where p was 1 and q was 0)

$M_{00} = 7$  (the number of attributes where p was 0 and q was 0)

$M_{11} = 0$  (the number of attributes where p was 1 and q was 1)

$$\text{SMC} = \frac{M_{11} + M_{00}}{M_{11} + M_{00} + M_{01} + M_{10}}$$

$$\text{Jaccard} = \frac{M_{11}}{M_{11} + M_{01} + M_{10}}$$

$$\text{Dice} = \frac{2M_{11}}{2M_{11} + M_{01} + M_{10}}$$



# Measures of similarity : Ordinal Variables

- Normalize Ranks
  - Normalize Rank; Treat as Numeric

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

- Look up table

	1	2	3
1	0	1	4
2	1	0	1
3	4	1	0



# Distance in multiple dimensions : Which distance measure to use?

- Gower Distance

- Idea: Use distance measure between 0 and 1 for each variable / dimension / feature  $d_{ij}^{(f)}$

- Aggregate:  $d(i, j) = \frac{1}{p} \sum_{i=1}^p d_{ij}^{(f)}$

- Variable-type specific distance measure

- Numeric Variables : Normalized Manhattan (L1 distance)  $d_{ij}^{(f)} = \frac{|x_{if} - x_{jf}|}{R_f}$ 
  - $x_{if}$ : Value for object i in variable f
  - $R_f$ : Range of variable f for all objects
- Categorical Variables : Dice coefficient
- Ordinal Variables: Rank Normalized



# Algorithms

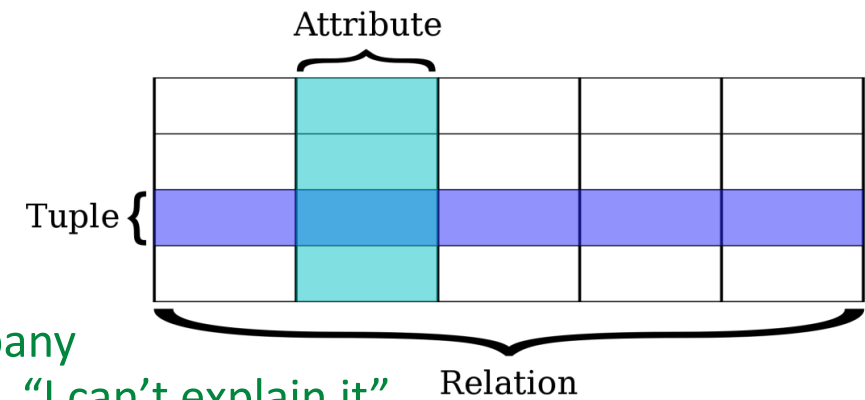
## Clustering



# Clustering 101

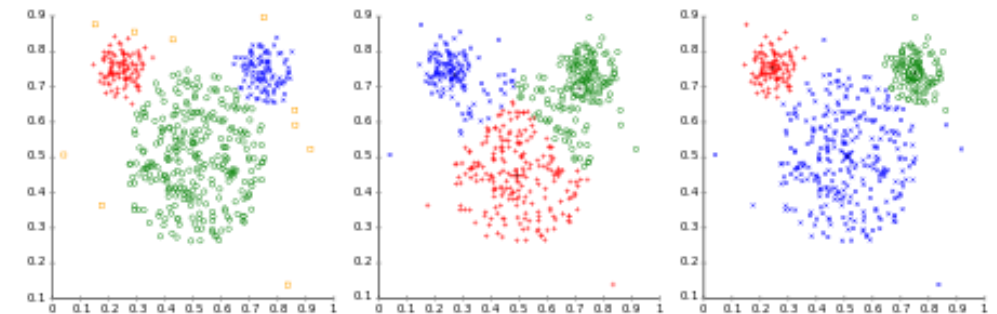
- Motivation

- Transaction data (Customer – Product matrix)
- Test measurements from a fab plant for chips
- Predict shipping weight of a package for a logistics company
- Segmentation, Pre-processing, Multimodal distributions, “I can’t explain it”



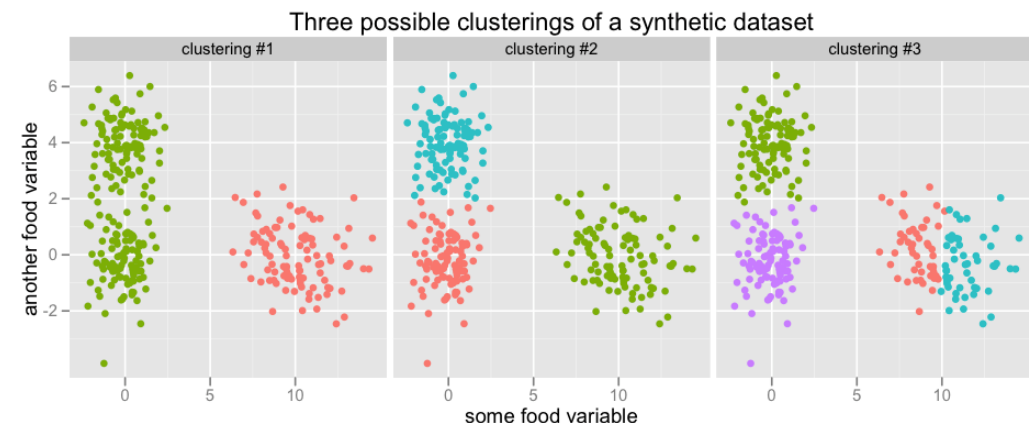
- Clustering

- Find elements (rows, tuples) which are similar.
- Finding “areas” in space where data is concentrated
- WYSIWYG : What You Select Is What You Get



- When are two elements / rows similar?

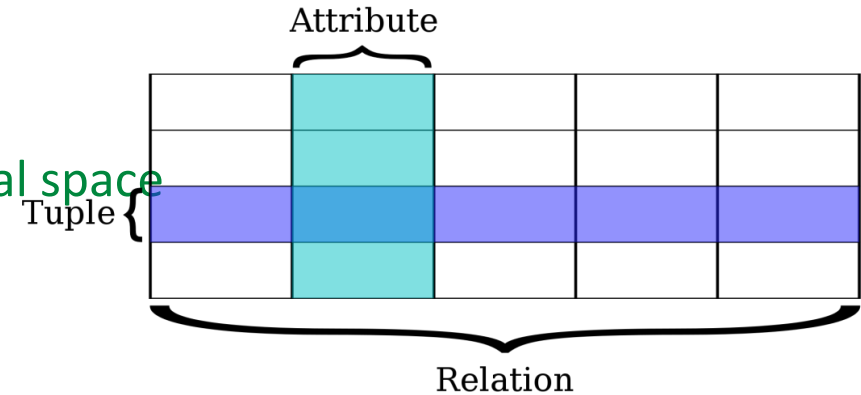
- A measure of (dis)similarity.
- Which dimensions (attributes) are relevant?
- Normalization?
- How many clusters?



# Dis-similarity / Distance based Clustering Framework

- Input

- Data
- Each data element (row, tuple) lives in a p-dimensional space
- A dis-(similarity) / distance measure  $d()$
- $k$  (Number of clusters)



$$X \in \mathbb{R}^{n \times p}$$

- Output

- $X$  partitioned into  $k$ -clusters;
- Cluster-id (colour) for each element (row, tuple)

$X$  partitioned into  $k$ -clusters; cluster-id for each  $\mathbf{x} \in X$   
 $C_1 \cup C_2 \cup \dots \cup C_k = \{1, 2, \dots, n\}$   
 $C_1 \cap C_2 \cap \dots \cap C_k = \phi$

- Measure

- Minimize within-sum-of-squares



# k-means

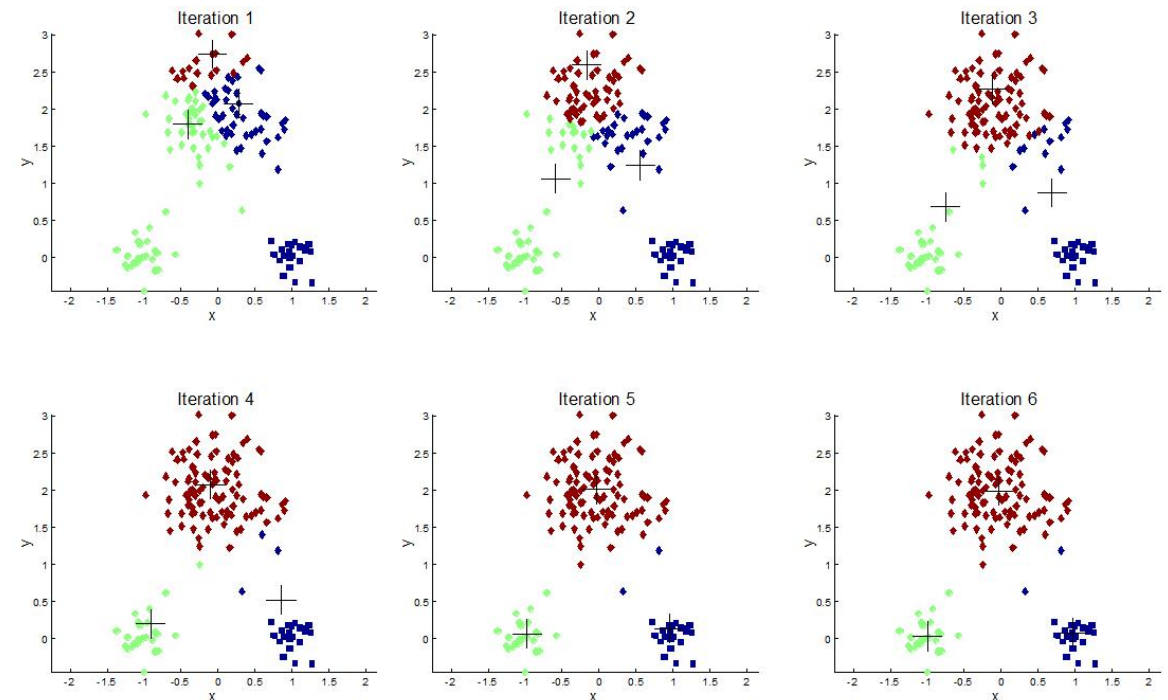
- Initialize
  - Pick k data points randomly from X : centroids
- Iterate
  - Assign each data point to the closest / most-similar centroid
  - For each cluster, update centroid
  - Repeat
- Terminate when “change in within cluster variation” < threshold
  - Amount by which elements in the same clusters are different

$$W(C_z) = \frac{1}{|C_z|} \sum_{i,j \in C_z} \|x_i - x_j\|_2^2$$
$$= \frac{1}{|C_z|} \sum_{i,j \in C_z} \sum_{d=1}^p (x_{id} - x_{jd})^2$$

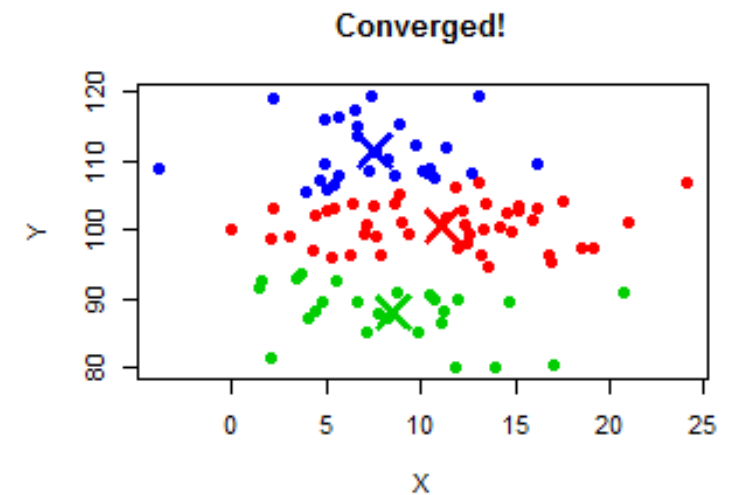
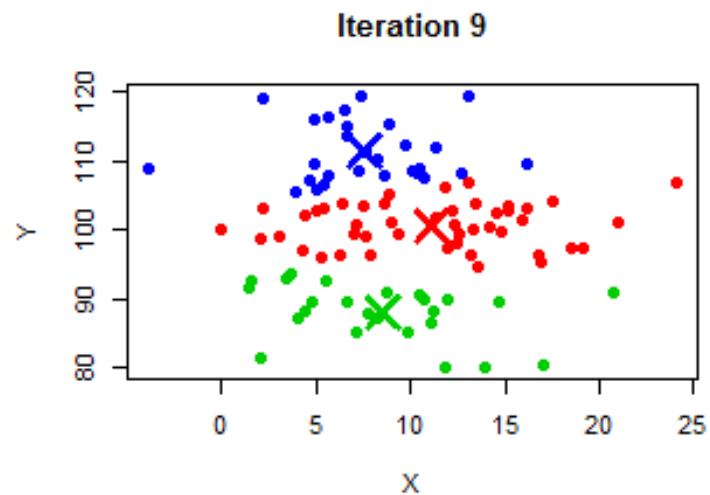
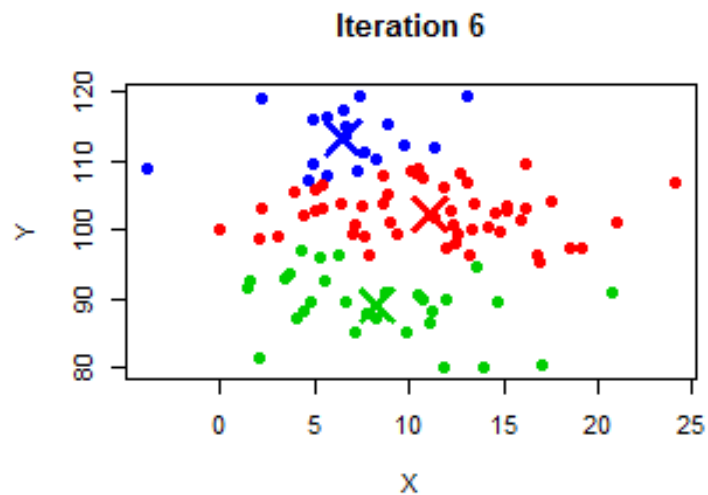
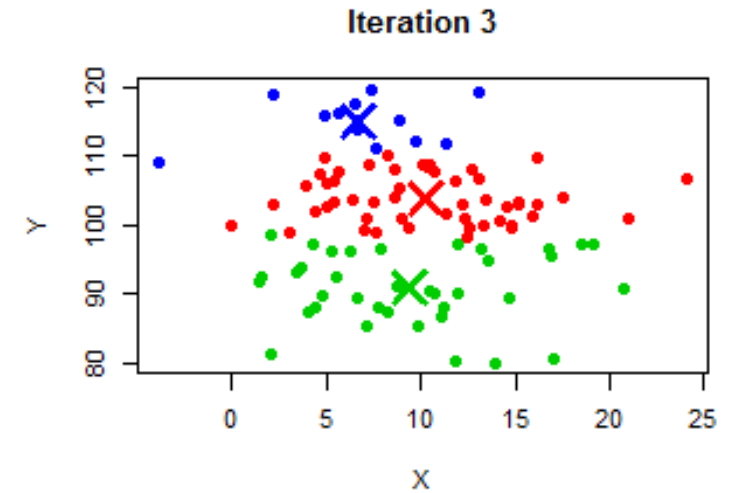
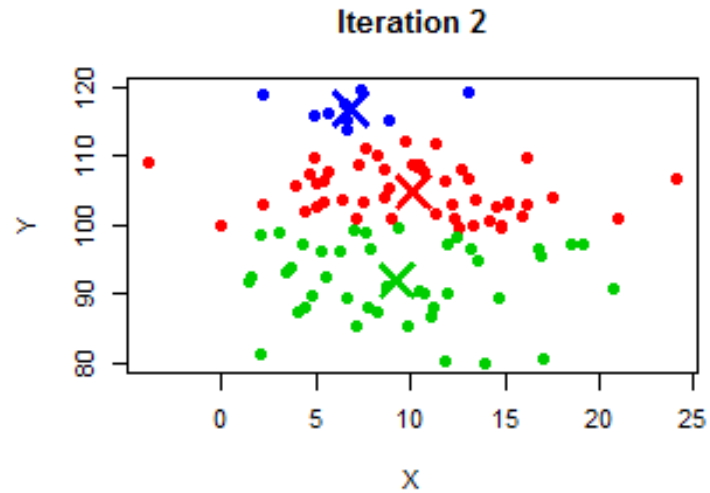
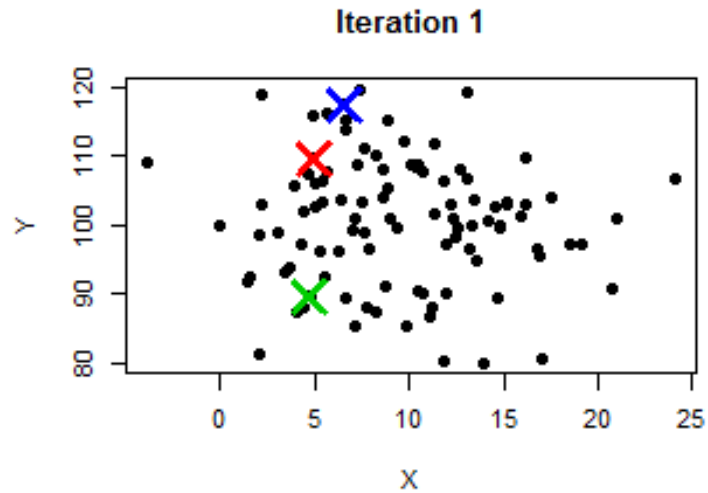
$$W(C) = \sum_{z=1}^k W(C_z)$$

## Algorithm k-means (k , D)

- 1 Choose random k data points as initial Clusters Mean ( cluster centers)
- 2 Repeat
- 3   For each data point x from D
- 4     Compute the distance between x and each cluster mean (centroid)
- 5     Assign x to the nearest cluster
- 6   End for
- 7   Re-compute the mean for current cluster collections
- 8 Until reaching stable clusters(current clusters means equals last clusters means)



# Are the clusters meaningful?





# Example

```
> (kc <- kmeans(newiris, 3))  
K-means clustering with 3 clusters of sizes 38, 50, 62
```

Cluster means:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
1	6.850000	3.073684	5.742105	2.071053
2	5.006000	3.428000	1.462000	0.246000
3	5.901613	2.748387	4.393548	1.433871

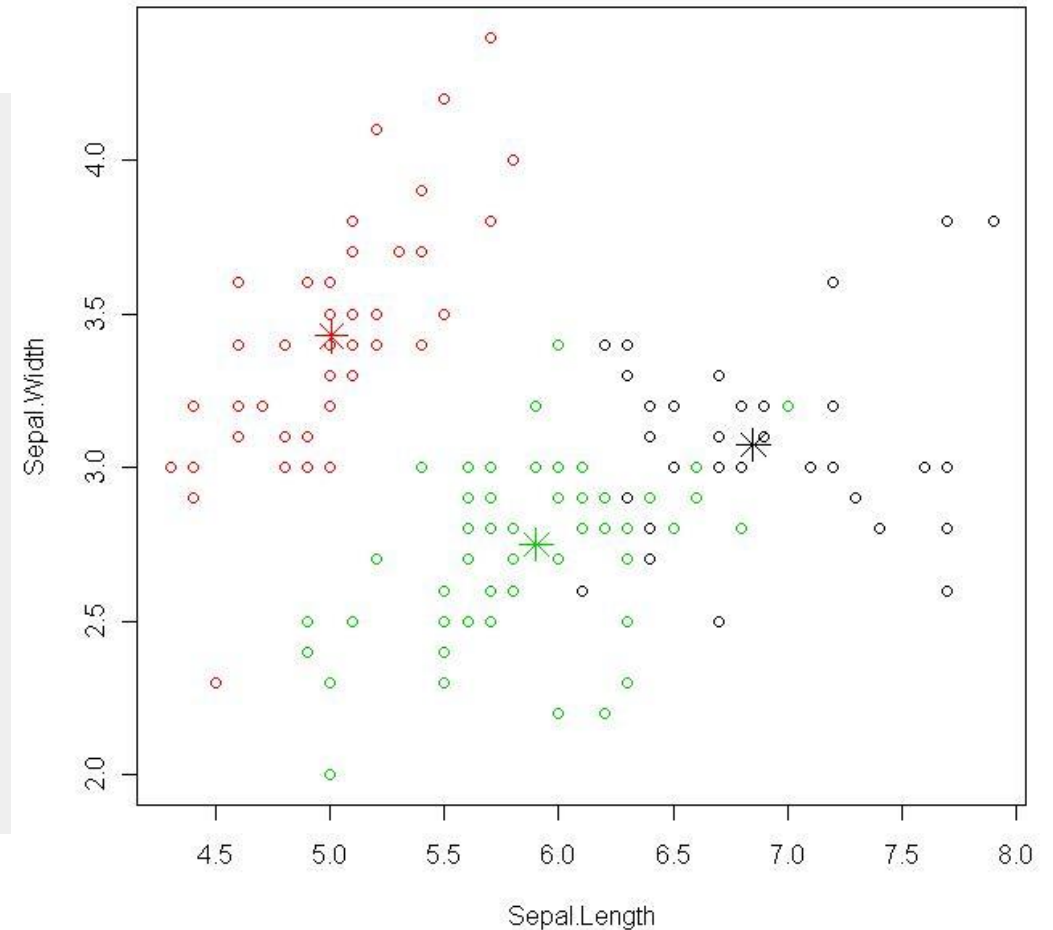
Clustering vector:

```
[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 2 2 2 2 2 2 2  
[30] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 1 3 3 3 3 3 3 3 3 3  
[59] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 1 3 3 3 3 3 3 3 3 3 3 3  
[88] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 1 3 1 1 1 1 1 3 1 1 1 1 1 1 3 3 1 1  
[117] 1 1 1 3 1 3 1 3 1 1 3 3 1 1 1 1 1 1 1 1 3 1 1 1 1 3 1 1 1 3 1 1  
[146] 1 3 1 1 3
```

Within cluster sum of squares by cluster:  
[1] 23.87947 15.15100 39.82097

Available components:

```
[1] "cluster" "centers" "withinss" "size"
```



```
> table(iris$Species, kc$cluster)
```

	1	2	3
setosa	0	50	0
versicolor	2	0	48
virginica	36	0	14

# Example

```
## 'data.frame':  30 obs. of  7 variables:
## $ rating      : num  43 63 71 61 81 43 58 71 72 67 ...
## $ complaints: num  51 64 70 63 78 55 67 75 82 61 ...
## $ privileges: num  30 51 68 45 56 49 42 50 72 45 ...
## $ learning   : num  39 54 69 47 66 44 56 55 67 47 ...
## $ raises     : num  61 63 76 54 71 54 66 70 71 62 ...
## $ critical   : num  92 73 86 84 83 49 68 66 83 80 ...
## $ advance    : num  45 47 48 35 47 34 35 41 31 41 ...
```

```
# Subset the attitude data
```

```
dat = attitude[,c(3,4)]
```

```
# Plot subset data
```

```
plot(dat, main = "% of favourable responses to  
Learning and Privilege", pch =20, cex =2)
```

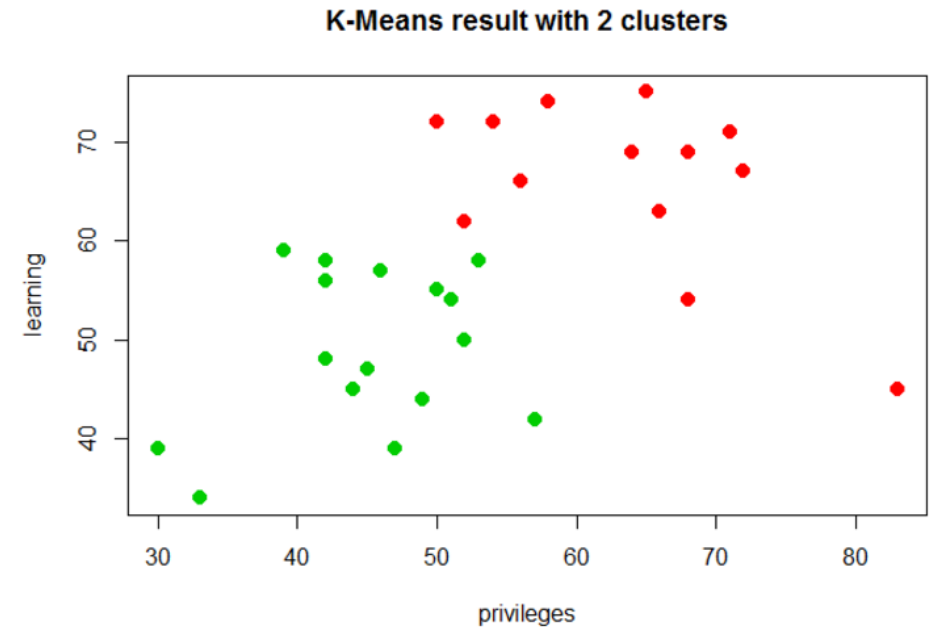
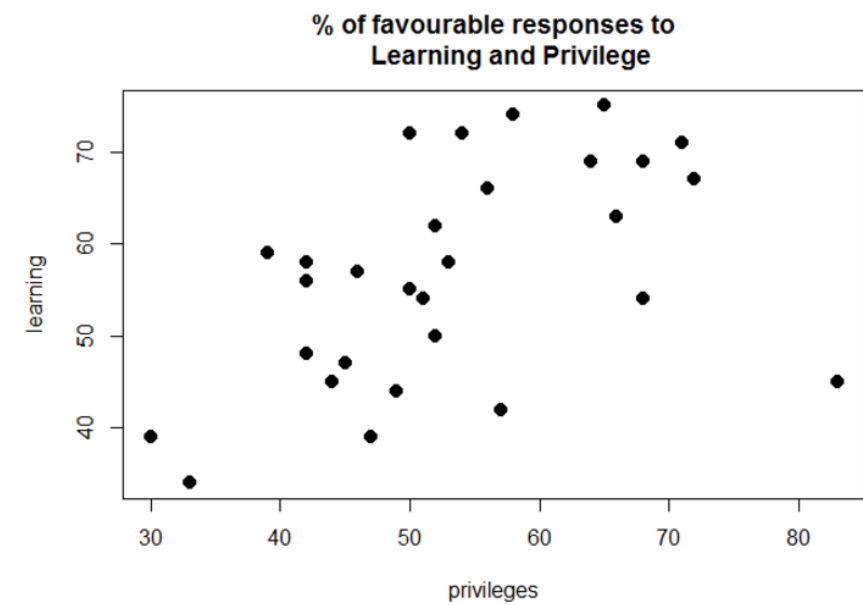
```
# Perform K-Means with 2 clusters
```

```
set.seed(7)
```

```
km1 = kmeans(dat, 2, nstart=100)
```

```
# Plot results
```

```
plot(dat, col =(km1$cluster +1) , main="K-Means result with 2 clusters", pch=20, cex=2)
```



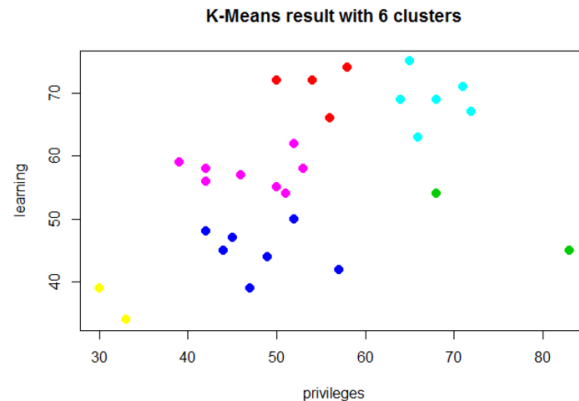
## Example (cont'd)

```
# Check for the optimal number of clusters given the data

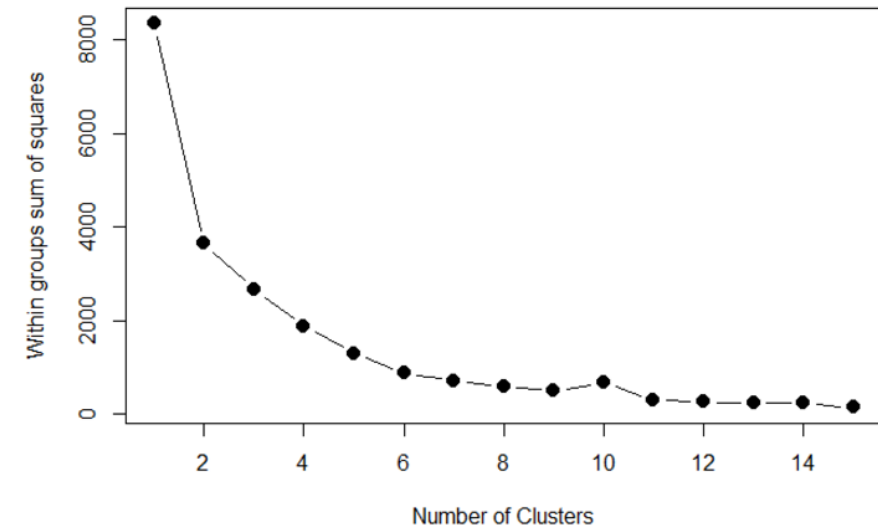
mydata <- dat
wss <- (nrow(mydata)-1)*sum(apply(mydata,2,var))
  for (i in 2:15) wss[i] <- sum(kmeans(mydata,
                                     centers=i)$withinss)
plot(1:15, wss, type="b", xlab="Number of Clusters",
     ylab="Within groups sum of squares",
     main="Assessing the Optimal Number of Clusters with the Elbow Method",
     pch=20, cex=2)
```

```
# Perform K-Means with the optimal number of clusters identified from the Elbow
set.seed(7)
km2 = kmeans(dat, 6, nstart=100)

# Examine the result of the clustering algorithm
km2
```



Assessing the Optimal Number of Clusters with the Elbow Method



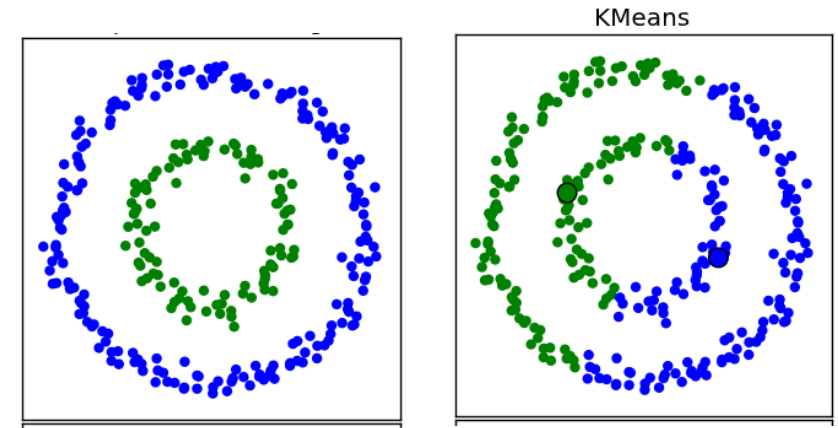
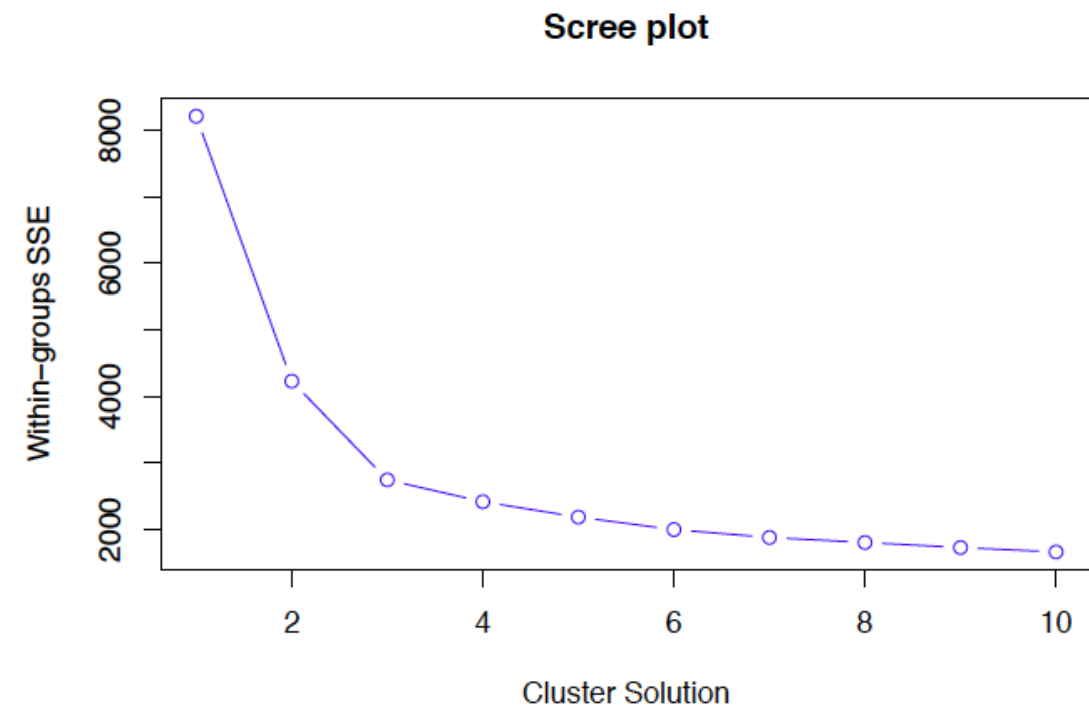
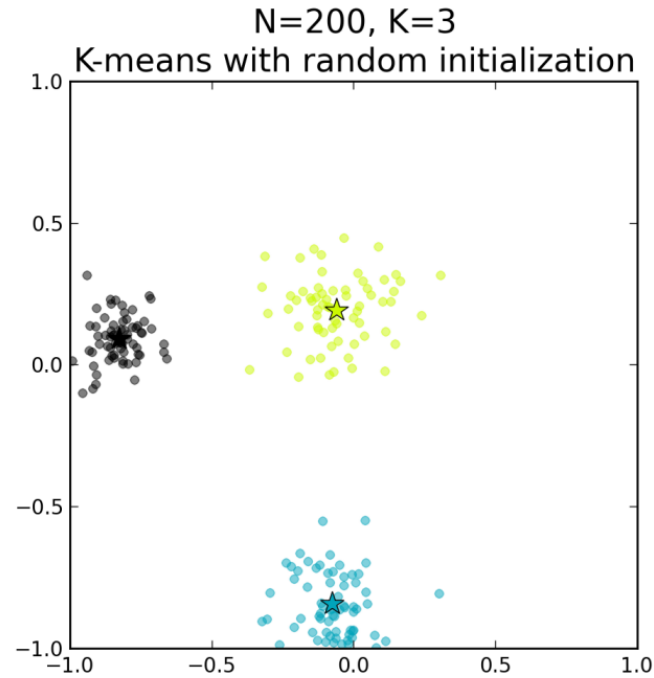
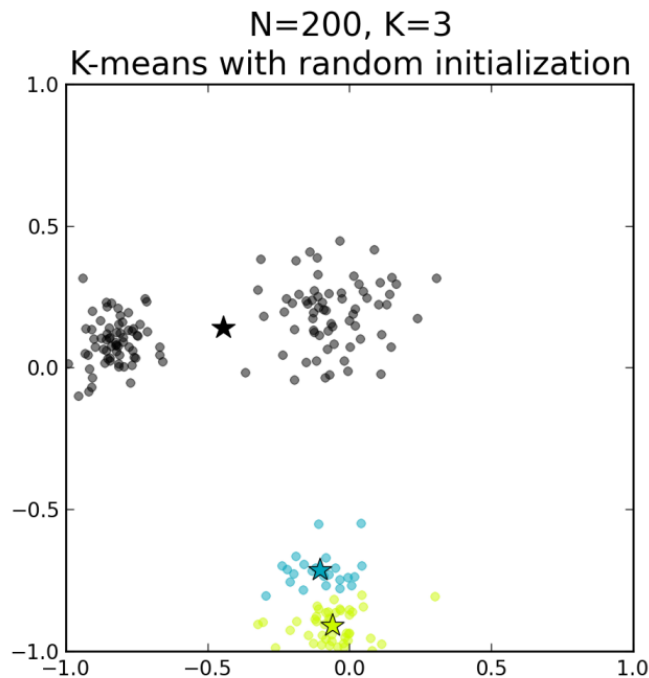
```
## K-means clustering with 6 clusters of sizes 4, 2, 8, 6, 8, 2
##
## Cluster means:
##   privileges learning
## 1  54.50000  71.000
## 2  75.50000  49.500
## 3  47.62500  45.250
## 4  67.66667  69.000
## 5  46.87500  57.375
## 6  31.50000  36.500
##
## Clustering vector:
## [1] 6 5 4 3 1 3 5 5 4 3 5 3 3 2 1 1 4 4 5 2 6 5 3 5 3 4 1 3 4 5
##
## Within cluster sum of squares by cluster:
## [1]  71.0000 153.0000 255.3750 133.3333 244.7500  17.0000
## (between_SS / total_SS =  89.5 %)
##
```

<https://rpubs.com/FelipeRego/K-Means-Clustering>



# Limitations of k-means

- Hyperparameter :  $k$ 
  - Not really a “limitation”
- Initial centroid at random
- Categorical (Mixed data?)
- Non-convex clusters



# k-means++

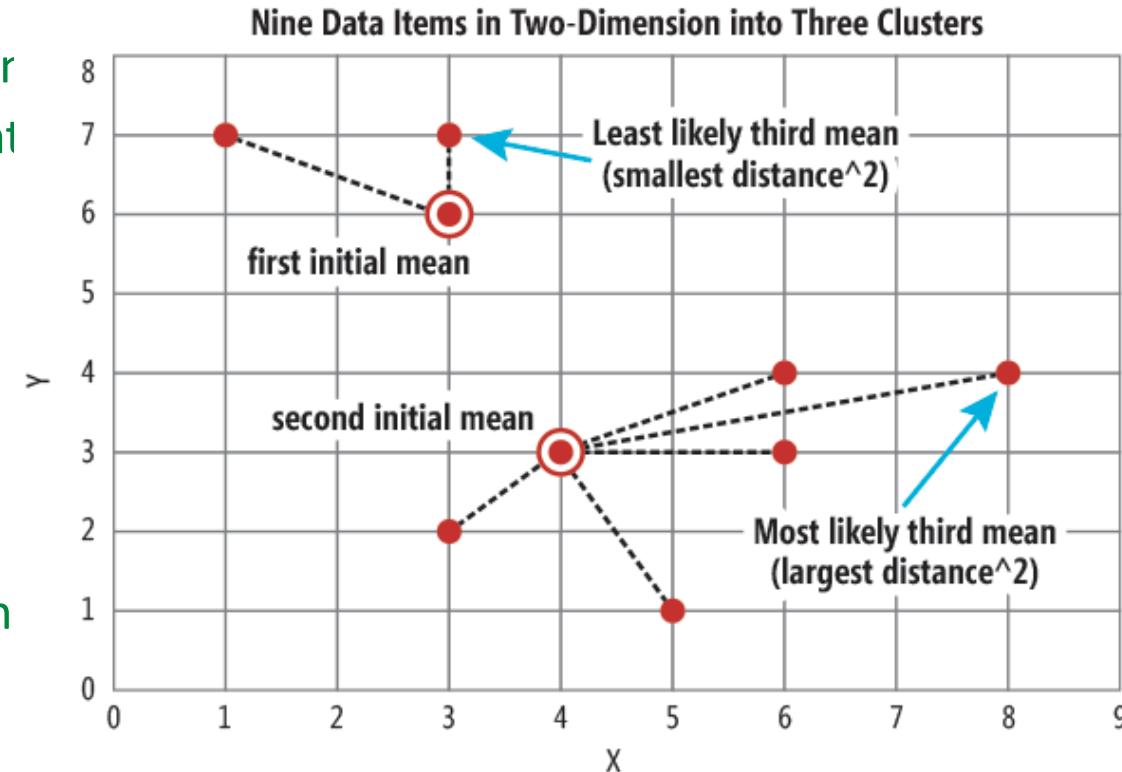
- Motivation

- Clusters in k-means depend on choice of initial centroids
- Each run (w/ different centroids) result in different clusters
- Can we do better?

- Key Idea: At Initialization,

- Pick first centroid at random
- For each  $x \in X$ ;  $g(x) = d(x; c_{\text{nearest}})$
- Pick  $x$  as next centroid with probability proportion to  $g(x)$
- Repeat till all  $k$  centroids are picked

- Use k means with these initial centroids



# Dealing with non-numeric data

- K-medoids
  - a.k.a. Partitioning around medoids (PAM)
- Takes custom distance matrix as input
  - e.g. output of a distance function (daisy() in R)
  - e.g. Gower distance metrics which works with mixed data type
- Uses median instead of mean to determine cluster centroids
  - a more *robust* estimate of a representative point than the mean
  - “Centroids” must be datapoints in the data set (medoids or exemplars)
- Computationally more expensive
- Others
  - Any clustering algorithm which takes dissimilarity (distance) matrix as input (hclust, dbscan)
  - Only categorical data : K-modes

## Algorithm k-means ( $k, D$ )

```
1 Choose random k data points as initial Clusters Mean (cluster centers)
2 Repeat
3   For each data point x from D
4     Compute the distance between x and each cluster mean (centroid)
5     Assign x to the nearest cluster
6   End for
7   Re-compute the mean for current cluster collections
8 Until reaching stable clusters (current clusters means equals last clusters
means)
```



# A measure for how good a clustering is

- Silhouette Value of an element

- Each element is assigned to a cluster (partitioning)
- A measure of how similar an element is to its own cluster compared to other clusters.
- Can be calculated with any distance / dis-similarity / similarity metric
- Normalized (Ranges from -1 to +1) → Interpretable
- High value (closer to +1) → An element is similar to other elements of its cluster
- cohesion  $a(i)$  to separation  $b(i)$  ratio
  - $a(i)$  : average dissimilarity of  $i$  with all other data within the same cluster
  - $b(i)_c$  : average dissimilarity of  $i$  with all other data in cluster  $c$
  - $b(i)$  : average dissimilarity of  $i$  with all other data in the 'neighboring' cluster =  $\min(b(i)_c)$
  - $s(i) \rightarrow 1 \rightarrow a(i) \ll b(i)$  and  $s(i) \rightarrow -1 \rightarrow a(i) \gg b(i)$

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

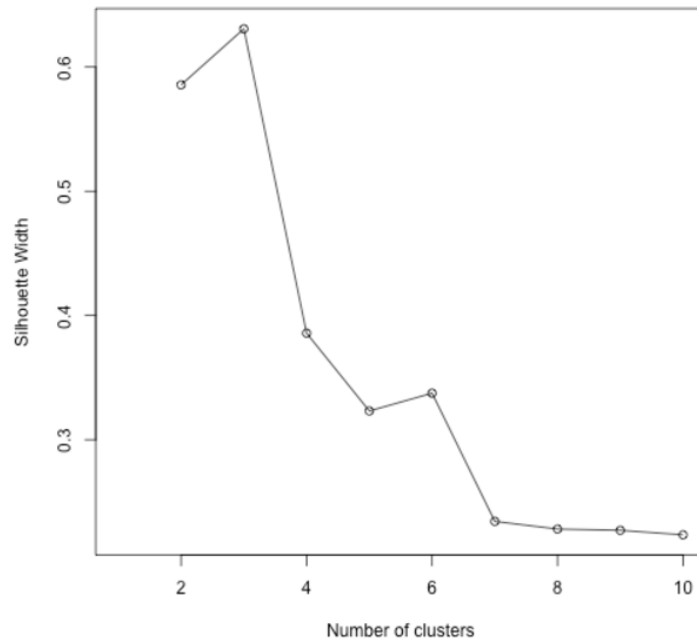
- Silhouette Value of a clustering

- Average silhouette value
- If most elements have a high value, clustering is “good”
- If most elements have a low value (→ -1) , clustering is “not good” → Try fewer / more clusters



# Example

- Continuous
  - Acceptance rate
  - Out of school tuition
  - Number of new students enrolled
- Categorical
  - Whether a college is public/private
  - Whether a college is “elite”



```
## Observations: 777
## Variables: 7
## $ name      (chr) "Abilene Christian University", "Ad...
## $ accept_rate (dbl) 0.7421687, 0.8801464, 0.7682073, 0....
## $ Outstate   (dbl) 7440, 12280, 11250, 12960, 7560, 13...
## $ Enroll     (dbl) 721, 512, 336, 137, 55, 158, 103, 4...
## $ Grad.Rate  (dbl) 60, 56, 54, 59, 15, 55, 63, 73, 80,...
## $ Private    (fctr) Yes, Yes, Yes, Yes, Yes, Yes, Yes,...
## $ isElite    (fctr) Not Elite, Not Elite, Not Elite, E...
```

```
gower_dist <- daisy(college_clean[, -1],
                    metric = "gower",
                    type = list(logratio = 3))

sil_width <- c(NA)

for(i in 2:10){

  pam_fit <- pam(gower_dist,
                 diss = TRUE,
                 k = i)

  sil_width[i] <- pam_fit$silinfo$avg.width

}
```

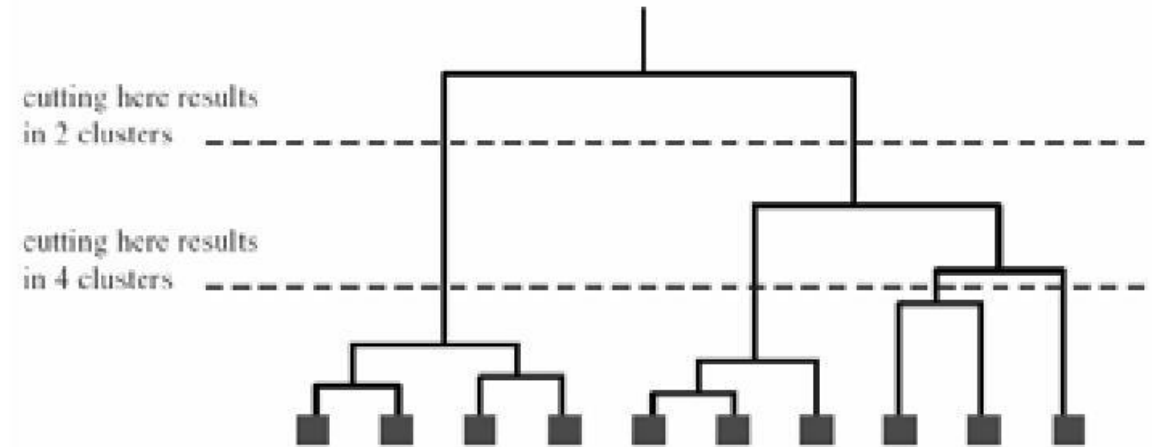
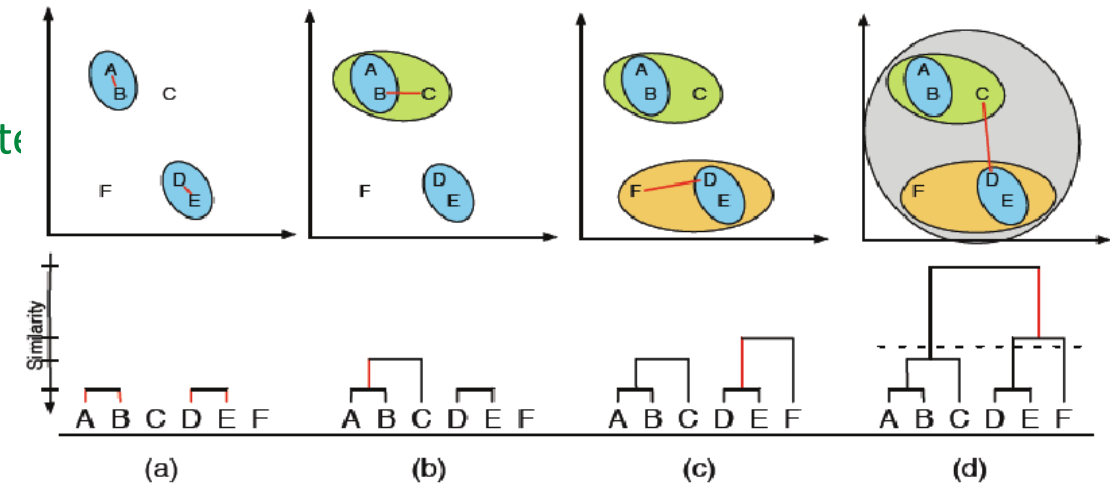




# Hierarchical

- Motivation
  - Instead of choosing  $k$  before clustering, choose it after
  - Key Idea: Build a hierarchy of clusters.
- Agglomerative : Bottom-Up
  - Initialize
    - Each element is a cluster
  - Iterate
    - Calculate all pairwise distance between clusters
    - Merge the two nearest clusters
    - Repeat
  - Terminate
    - When all clusters merge into one.
    - Output dendrogram : let user choose  $k$
- Divisive : Top-Down
  - Reverse
- Distance between clusters?

## Example: Hierarchical Agglomerative Clustering



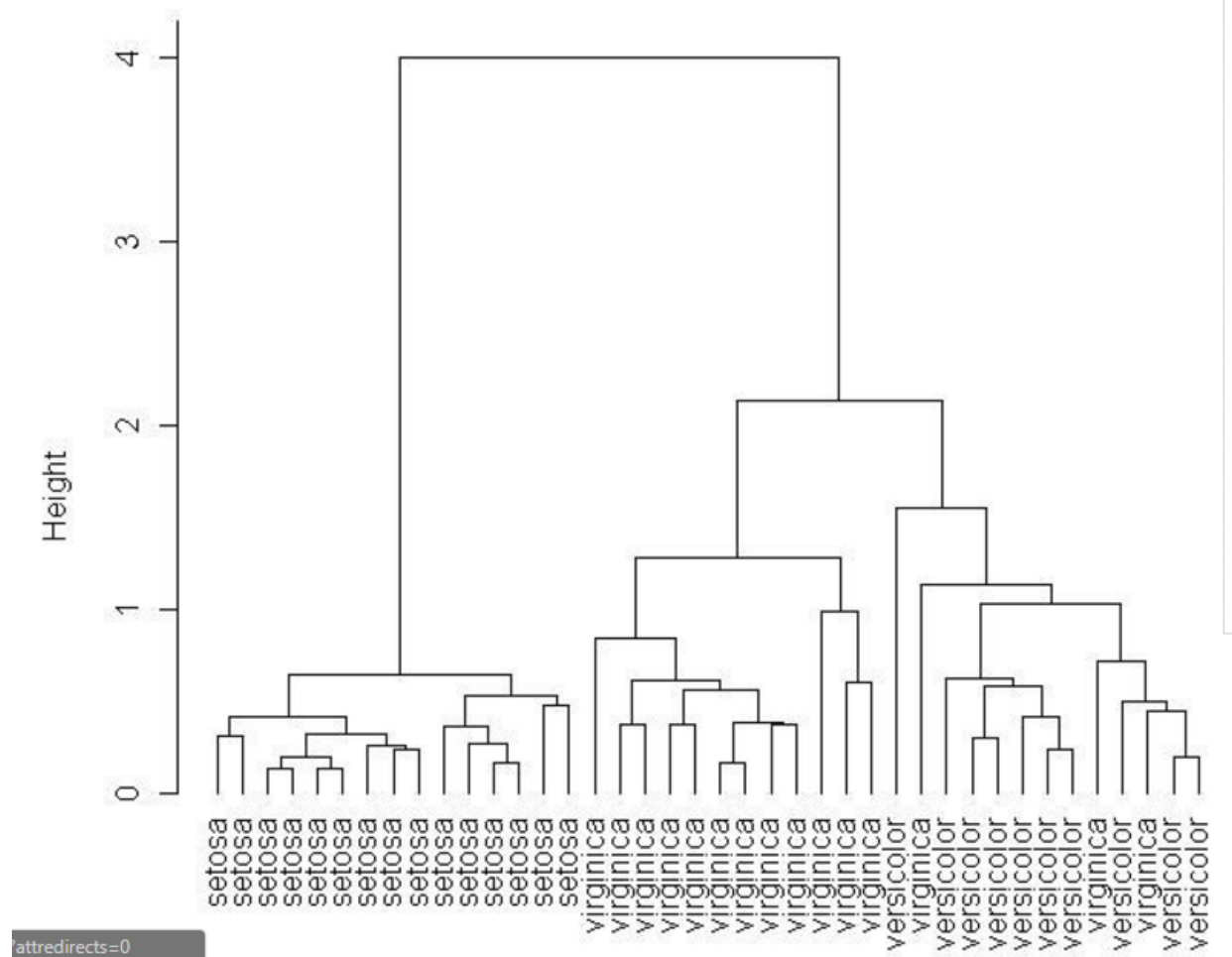
# Distance between clusters?

- Maximum or complete linkage clustering:
  - Max (all pairwise distances)
  - Tends to produce more compact clusters.
- Minimum or single linkage clustering:
  - Min (all pairwise distances)
  - Tends to produce long, “loose” clusters.
- Mean or average linkage clustering
  - Ave (all pairwise distances)
- Centroid linkage clustering:
  - Distance (Dissimilarity) between the centroid for cluster 1 and the centroid for cluster 2.
- Ward's minimum variance method
  - Minimizes the total within-cluster variance.
  - At each step the pair of clusters with minimum between-cluster distance are merged.



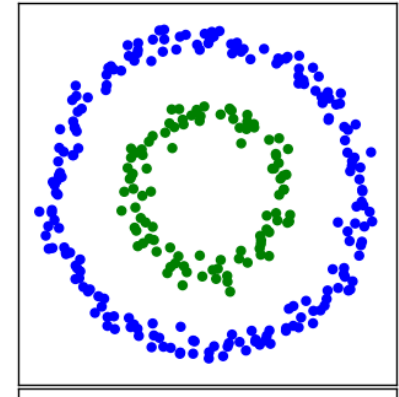
# Example

```
> hc <- hclust(dist(irisSample), method="ave")  
> plot(hc, hang = -1, labels=iris$Species[idx])
```



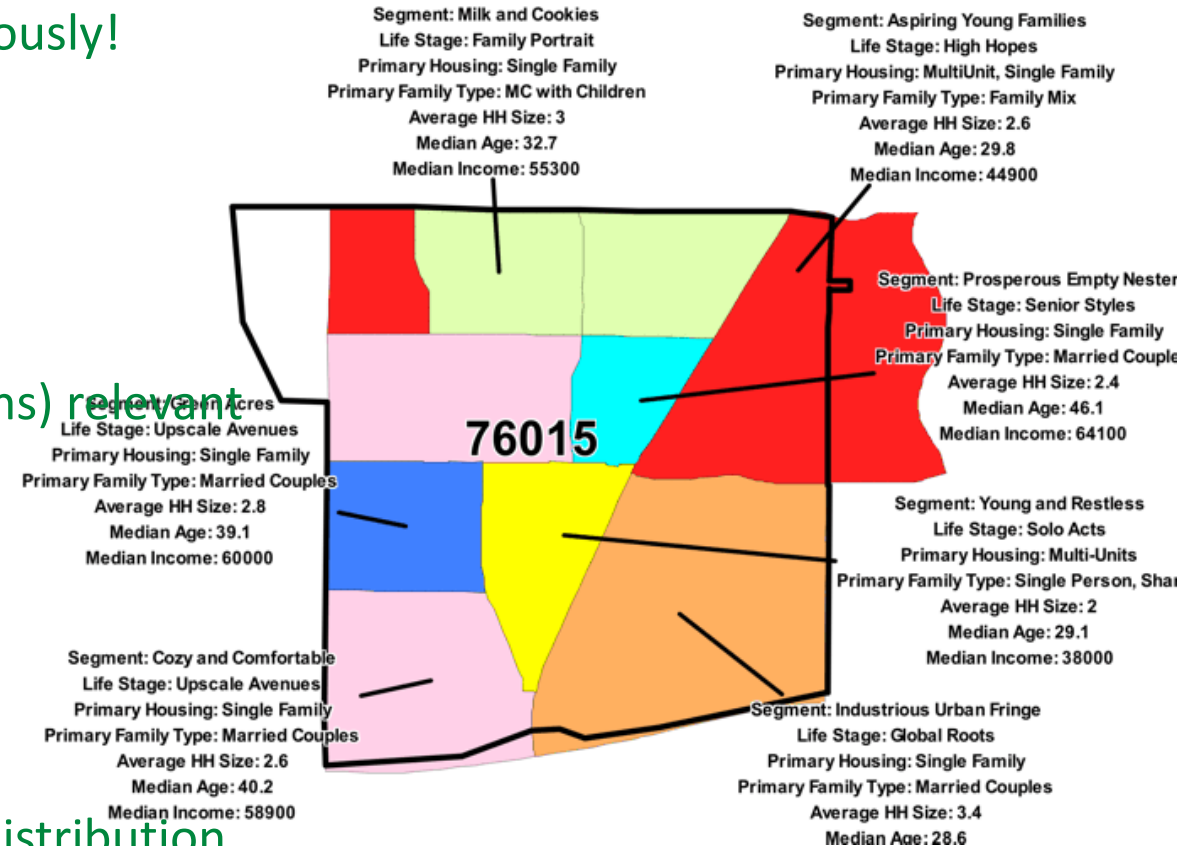
# DBScan

- Motivation
  - Some data does not lend itself into centroid-based clustering
- Key Idea
  - Use “density” as the defining characteristic
  - Partition points into dense regions separated by not-so-dense regions
  - What is dense?
    - Density at a point : # of points within a circle of radius  $\epsilon$
    - Dense region: A circle of radius  $\epsilon$  that contains at-least  $m$  points
- Iterate
  - i. Pick a data point, that has not been visited, randomly from  $X$
  - ii. If number of points within  $\epsilon > m$ , create a cluster; otherwise label it as noise
    - i. For each point in this new cluster, repeat (ii)
  - iii. Repeat till all points are exhausted
- Cluster
  - All points within the cluster are mutually density-connected (reachable by paths with each hop  $< \epsilon$ )

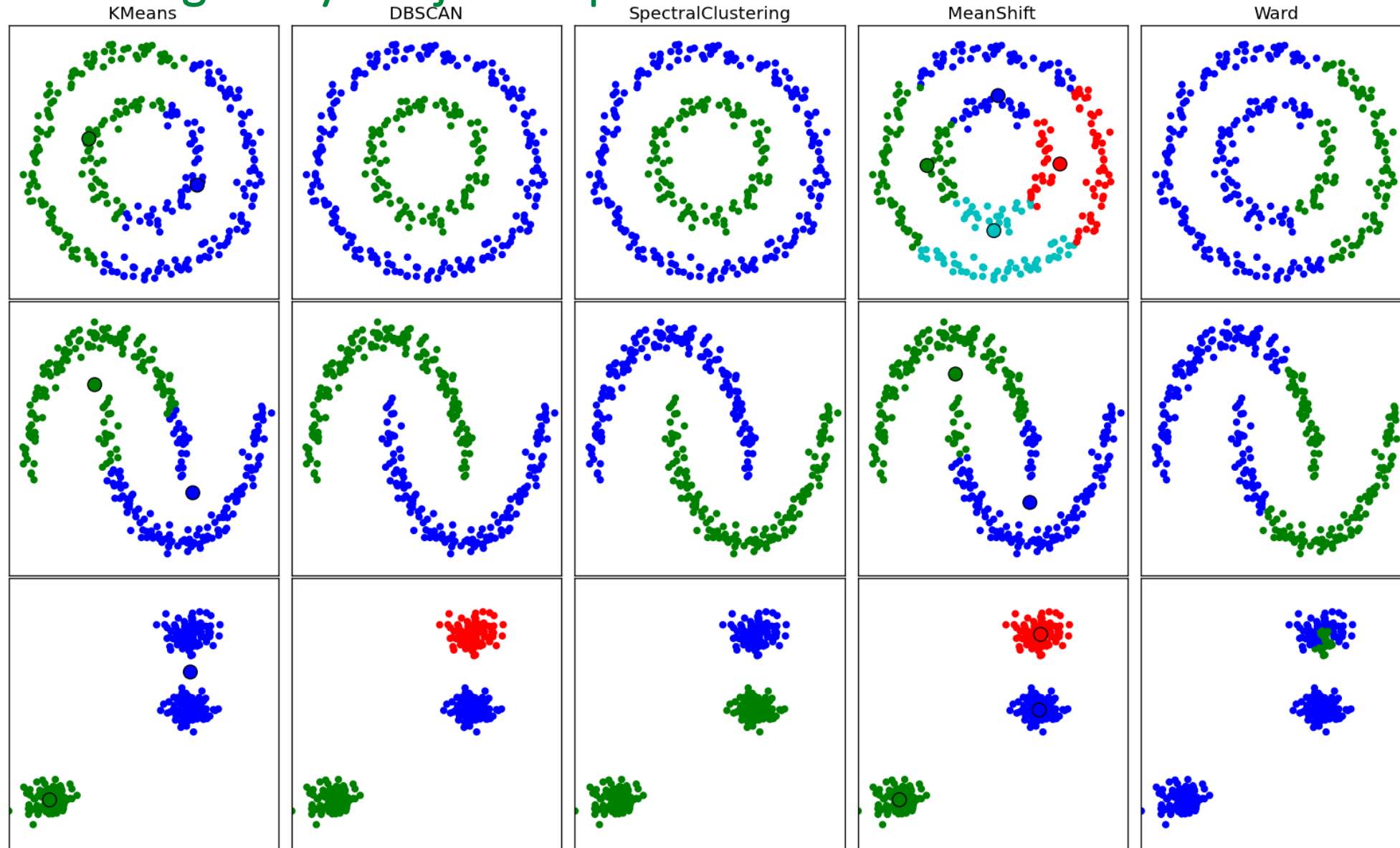


# Clustering : Gotchas!

- Powerful tool
  - Will ALWAYS give you some clusters : Use cautiously!
  - What is a “good” clustering?
  - Unsupervised Learning
- Pre-processing
  - Choose relevant features (attributes, dimensions) relevant
  - Choose (dis-)similarity / distance metric
  - Normalize variables (or not)
  - These choices impact which clusters emerge
- Post-processing
  - Characterize each clusters in terms of feature distribution
  - Name your clusters



# Clustering : Why not just stop here?



# Q?

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Insofe

