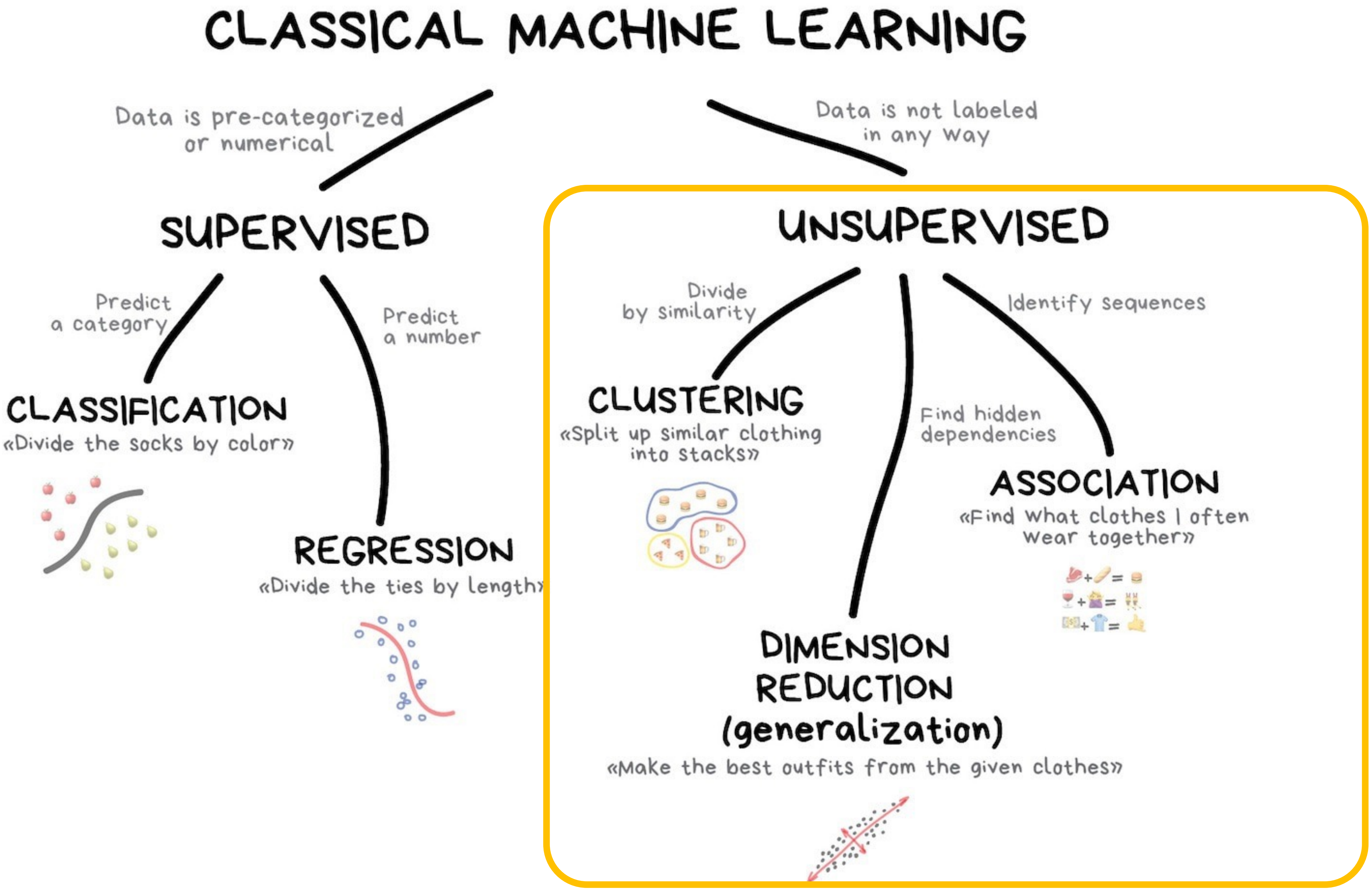
Clustering

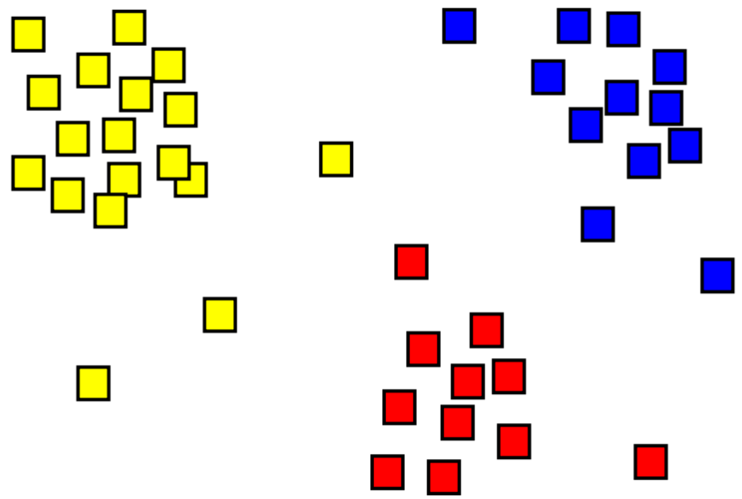
Type of Learning



Clustering

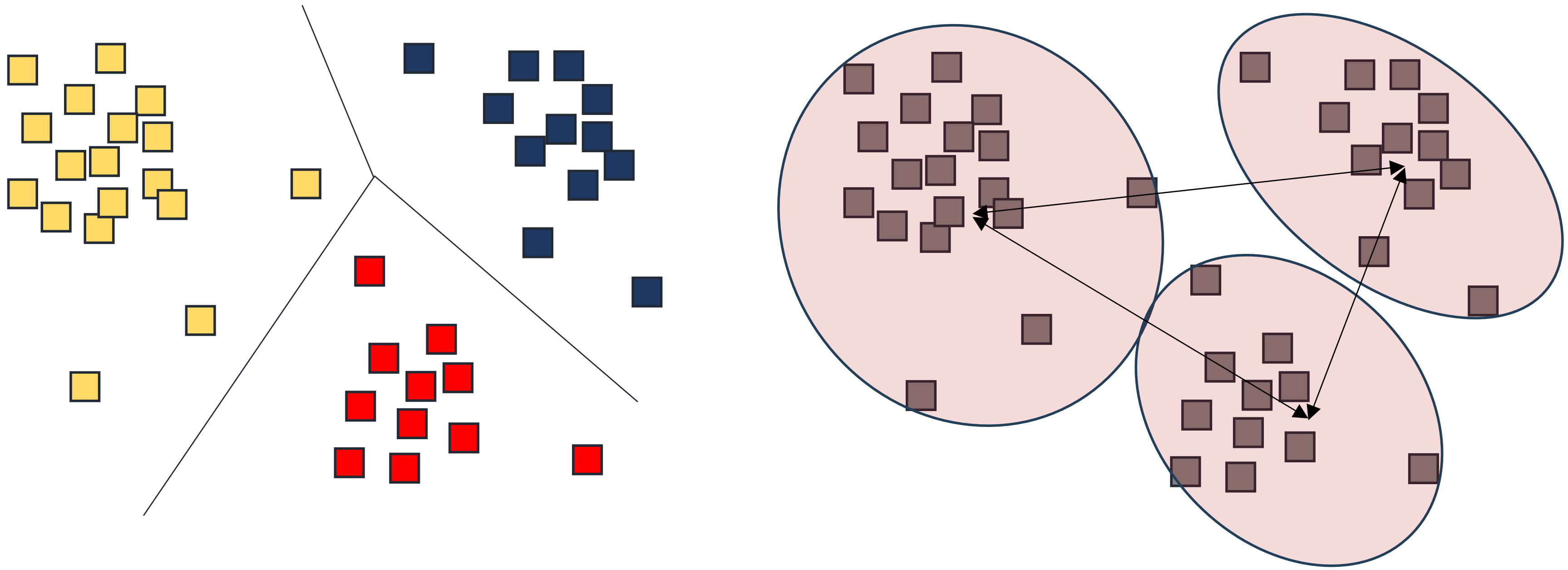
Unsupervised Learning: Clustering

- **Clustering is to group a set of data points to satisfy following conditions as much as possible**
  - Data points in the same group are more similar to each other than to data points in other groups



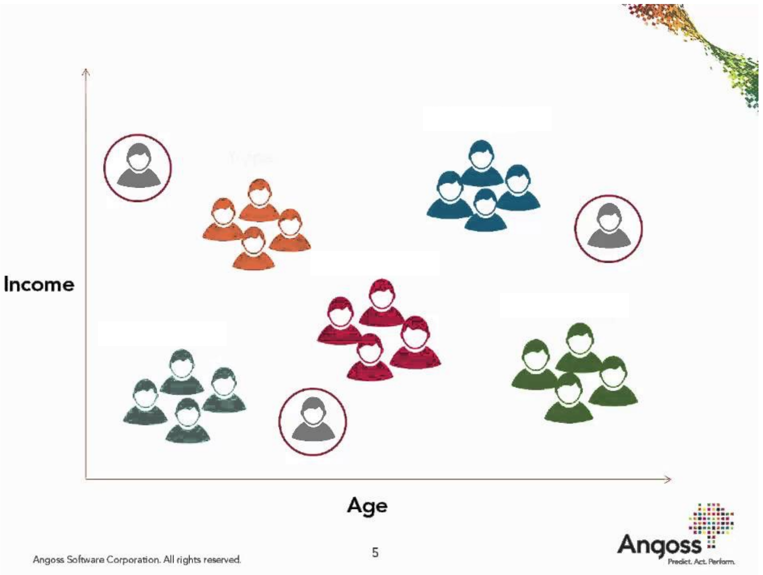
Unsupervised Learning: Clustering

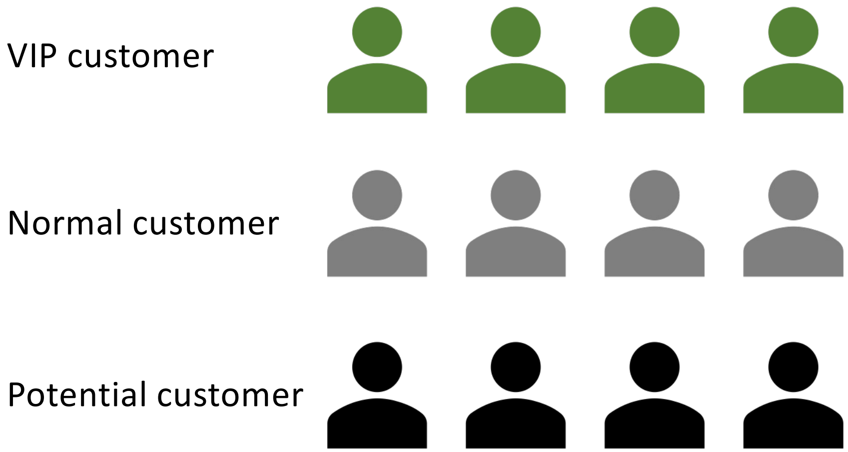
- **Classification vs. Clustering**
  - Classification: Classification involves dividing data into pre-defined categories or classes based on their features.
  - Clustering: Clustering involves grouping unlabeled data points into clusters based on their similarity or proximity to each other.



Clustering Application

- **Example. Customer segmentation**
  - Customer segmentation categorize customers into different groups for targeted marketing.
    - ✓ For example, young customers with higher income might be targeted with luxury or technology products while old customers with lower income with budget-friendly and traditional offerings.
  - RFM analysis
    - ✓ RFM analysis divides customers based on three factors: Recency, Frequency, and Monetary value.





Clustering

- **Data points in the same group are more similar to each other than to data points in other groups**

1. How to know some points are more similar than others?
→ Using a distance measure

2. How to group?
→ Determine certain rule to group (Clustering algorithm)

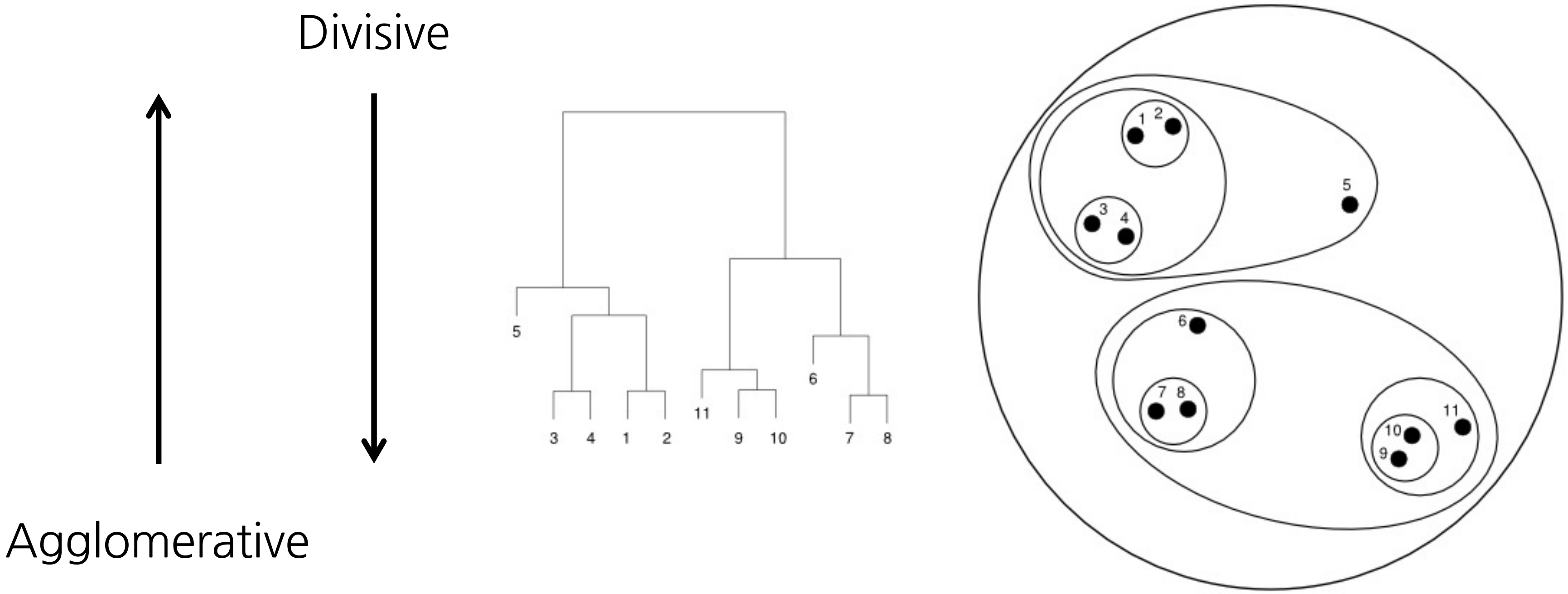
3. How to decide the number of groups or how to evaluate?
→ Evaluation metrics for clustering

Hierarchical Clustering

k-Means Clustering

Hierarchical Clustering

- **Hierarchical clustering builds a hierarchy of clusters**
  - Agglomerative: Bottom-up approach, each data point starts in its own cluster and pairs of clusters are merged as one moves up the hierarchy
  - Divisive: Top-down approach, all data points start in one cluster and splits are performed recursively as one moves down the hierarchy



Linkage Criteria for Agglomerative Clustering

- **Way to calculate similarity between two clusters A, B**

Type	Formula
Complete-linkage	$\max\{d(a,b) : a \in A, b \in B\}$
Single-linkage	$\min\{d(a,b) : a \in A, b \in B\}$
Mean linkage	$\frac{1}{\lvert A\rvert \lvert B\rvert} \sum_{a \in A} \sum_{b \in B} d(a,b)$
Centroid linkage	$d(c_A, c_B)$
Ward linkage	$\mathrm{Var}(A \cup B) - \mathrm{Var}(A) - \mathrm{Var}(B)$

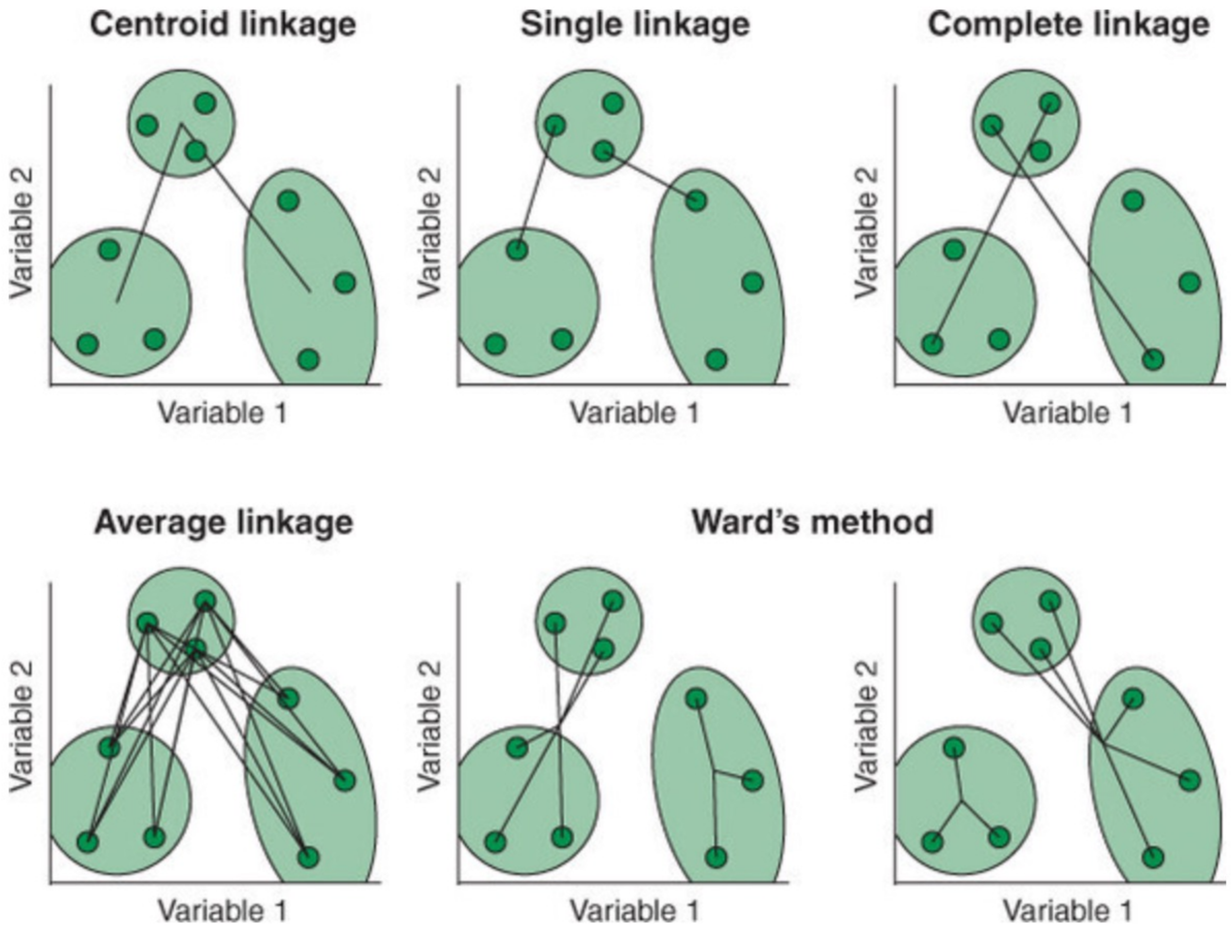
- a belongs to A, b belongs to B
- $\mathrm{Var}(X)$ is within-cluster variance (variance of cluster X)

$$Var(X) = \frac{1}{n_A} \sum_{i \in A} \lVert \mathbf{x}_i - \mu_A \rVert^2$$

- $d(a,b)$ is distance between two data points a and b

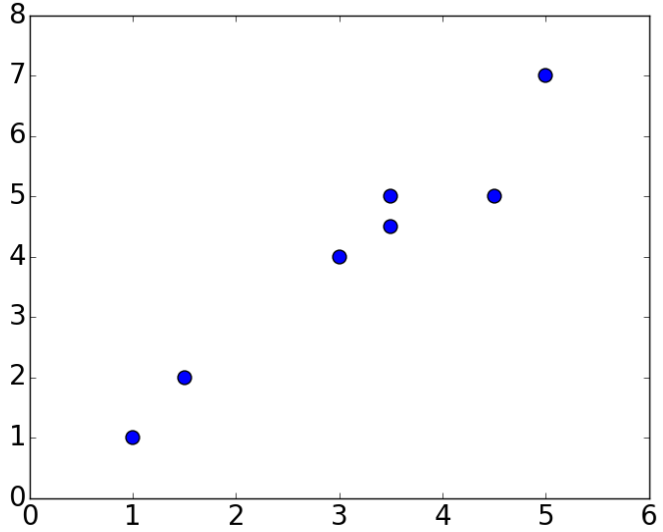
Linkage Criteria for Agglomerative Clustering

- **Way to calculate similarity between two clusters A, B**



Question

- **Clustering for 2D dataset**



	1	2	3	4	5	6	7
x	1.0	1.5	3.0	5.0	3.5	4.5	3.5
y	1.0	2.0	4.0	7.0	5.0	5.0	4.5
C	1	1	2	2	2	2	2

- 1) Using complete-linkage, calculate linkage criterion of cluster 1 and 2

- 2) Using centroid-linkage, calculate linkage criterion of cluster 1 and 2

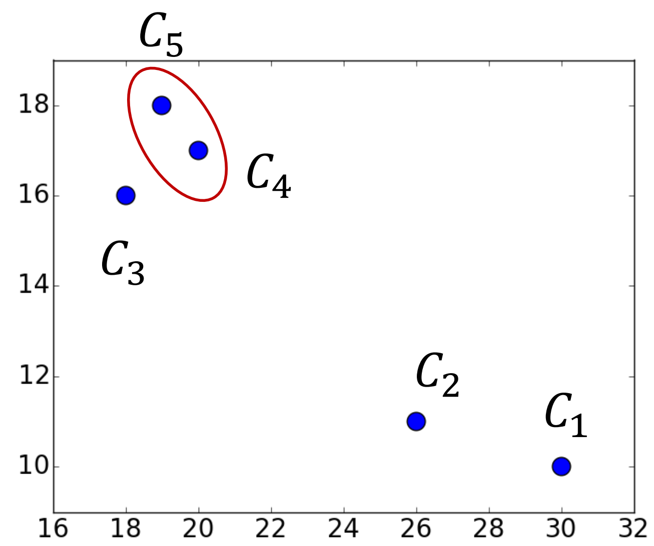
Example: Single Linkage Clustering

- **Find clusters through single linkage hierarchy clustering**
  - Start each data as own cluster
  - Distance measure between two points: Euclidean distance

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Distance $d(A,B) = \min\{d(a,b): a \in A, b \in B\}$

	1	2	3	4	5
1	0				
2	4.12	0			
3	15.23	11.18	0		
4	12.21	8.48	4.12	0	
5	13.60	9.90	3.61	**1.41**	0



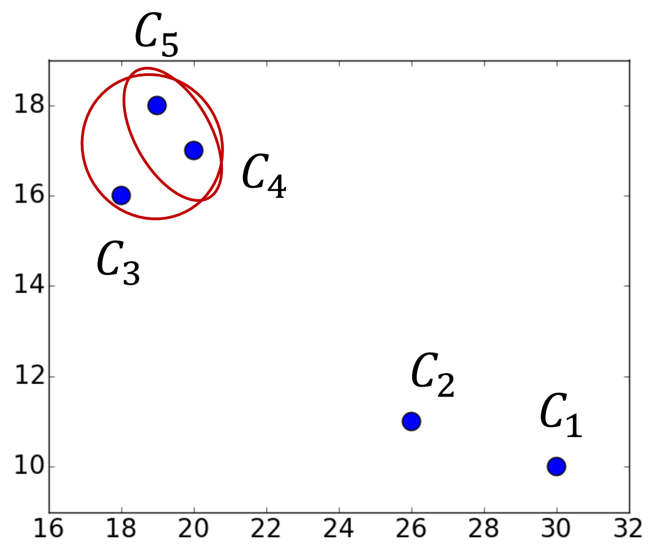
Example: Single Linkage Clustering

- **Find clusters through single linkage hierarchy clustering**
  - Merge cluster 4 and 5 to create new cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Distance $d(A,B) = \min\{d(a,b): a \in A, b \in B\}$

	1	2	3	6
1	0			
2	4.12	0		
3	15.23	11.18	0	
6	12.21	8.48	**3.61**	0



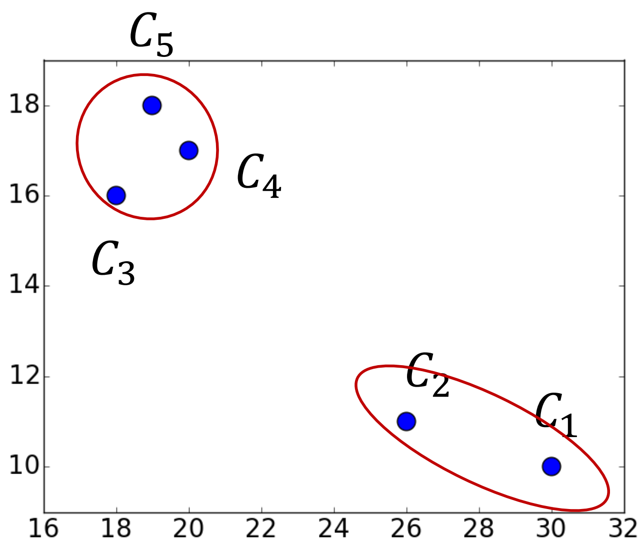
Example: Single Linkage Clustering

- **Find clusters through single linkage hierarchy clustering**
  - Merge cluster 3 and 6 to create new cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Distance $d(A, B) = \min\{d(a, b): a \in A, b \in B\}$

	1	2	7
1	0		
2	**4.12**	0	
7	12.21	8.48	0



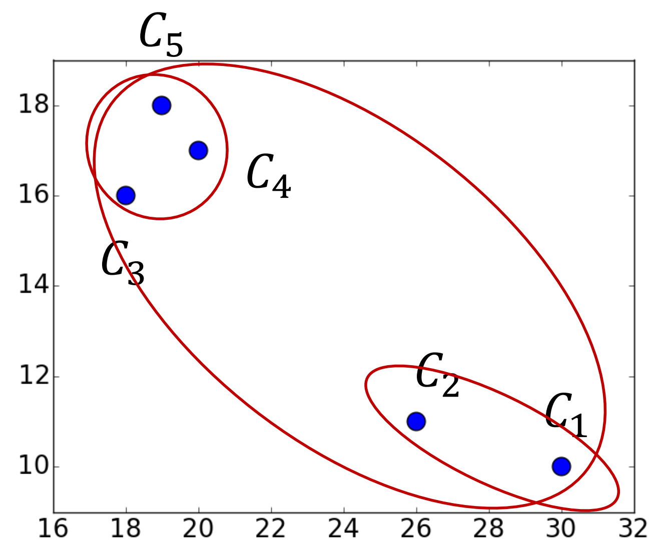
Example: Single Linkage Clustering

- **Find clusters through single linkage hierarchy clustering**
  - Merge cluster 1 and 2 to create new cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

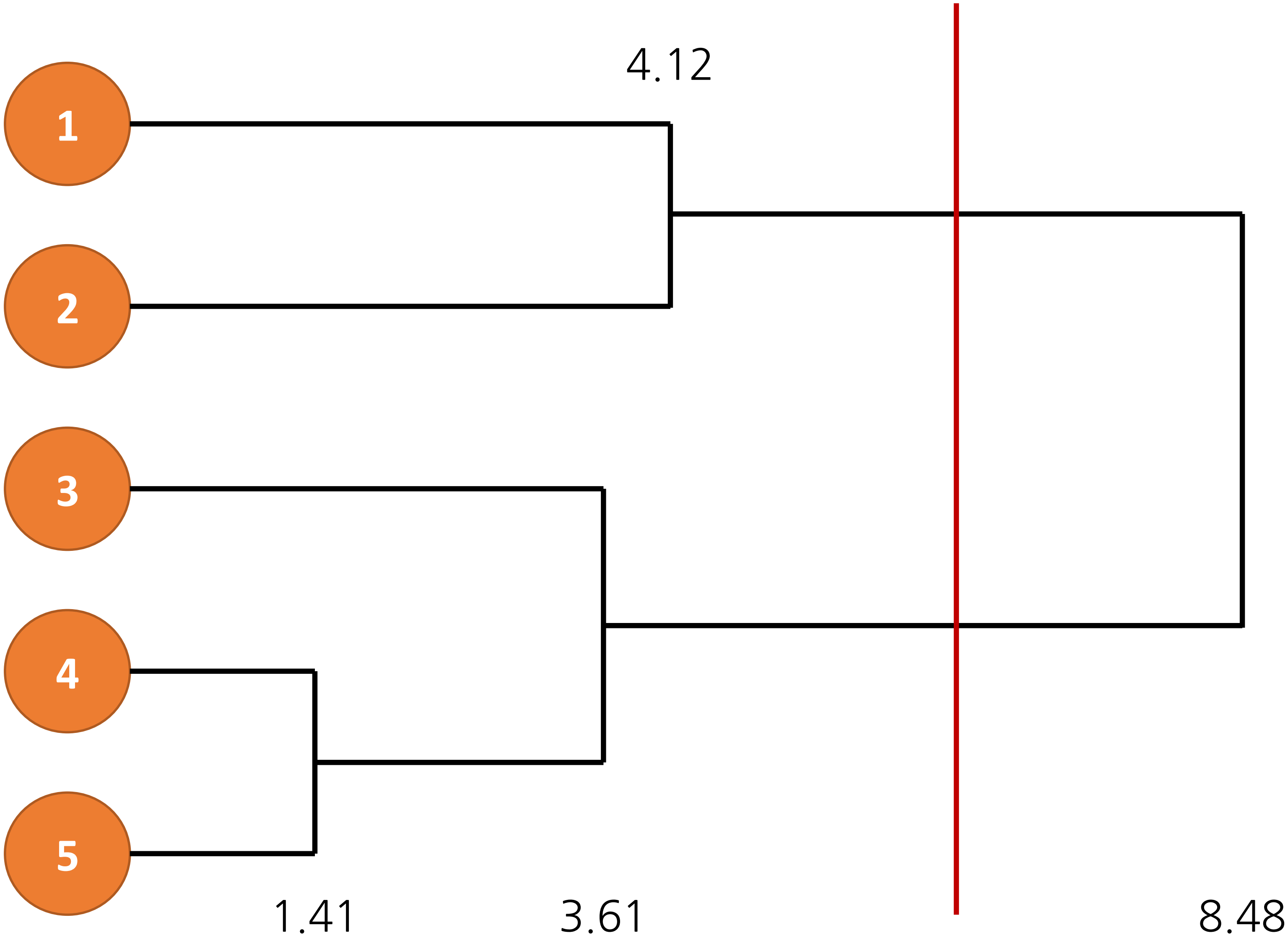
Distance $d(A, B) = \min\{d(a, b): a \in A, b \in B\}$

	7	8
7	0	
8	8.48	0



Example: Single Linkage Clustering

- **Dendrogram**



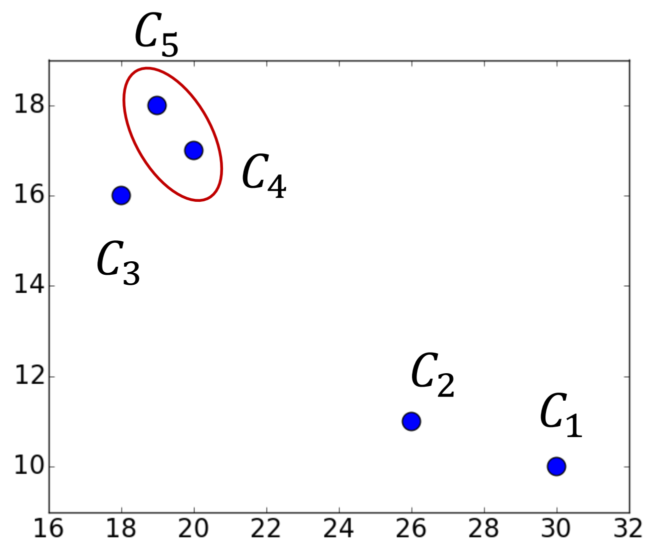
Example: Complete Linkage Clustering

- **Find clusters through complete linkage hierarchy clustering**
  - Start each data as own cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Distance $d(A,B) = \max\{d(a,b): a \in A, b \in B\}$

	1	2	3	4	5
1	0				
2	4.12	0			
3	15.23	11.18	0		
4	12.21	8.48	4.12	0	
5	13.60	9.90	3.61	**1.41**	0



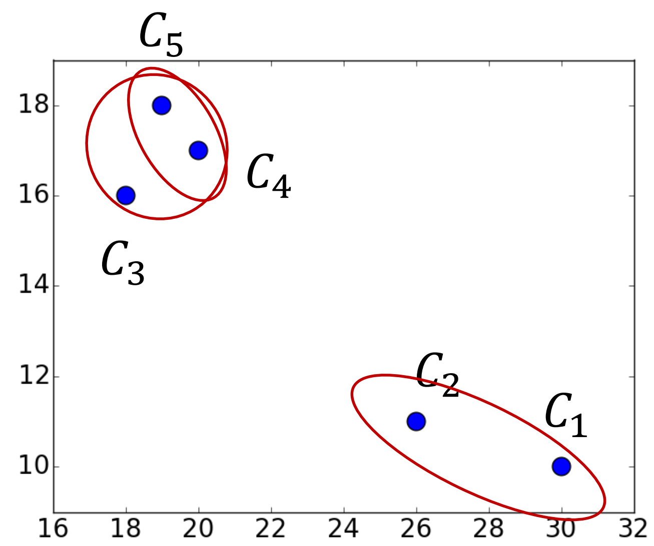
Example: Complete Linkage Clustering

- **Find clusters through complete linkage hierarchy clustering**
  - Merge cluster 4 and 5 to create new cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Distance $d(A, B) = \max\{d(a, b) : a \in A, b \in B\}$

	1	2	3	6
1	0			
2	**4.12**	0		
3	15.23	11.18	0	
6	13.60	9.90	**4.12**	0



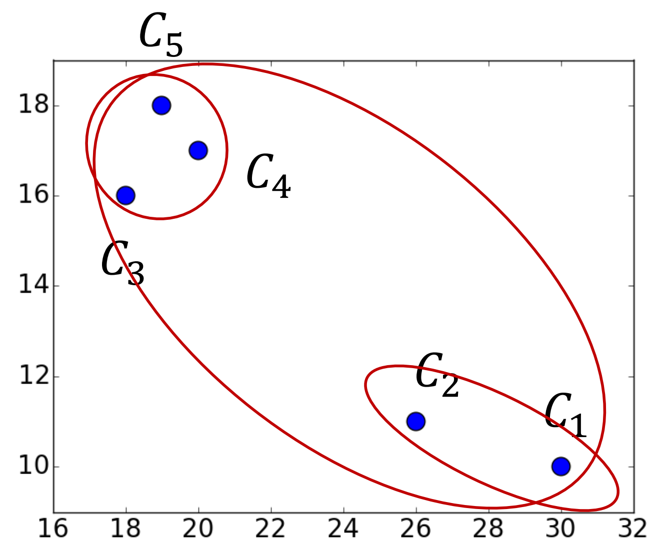
Example: Complete Linkage Clustering

- **Find clusters through complete linkage hierarchy clustering**
  - Merge cluster 1 and 2 to create new cluster
  - Merge cluster 3 and 6 to create new cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

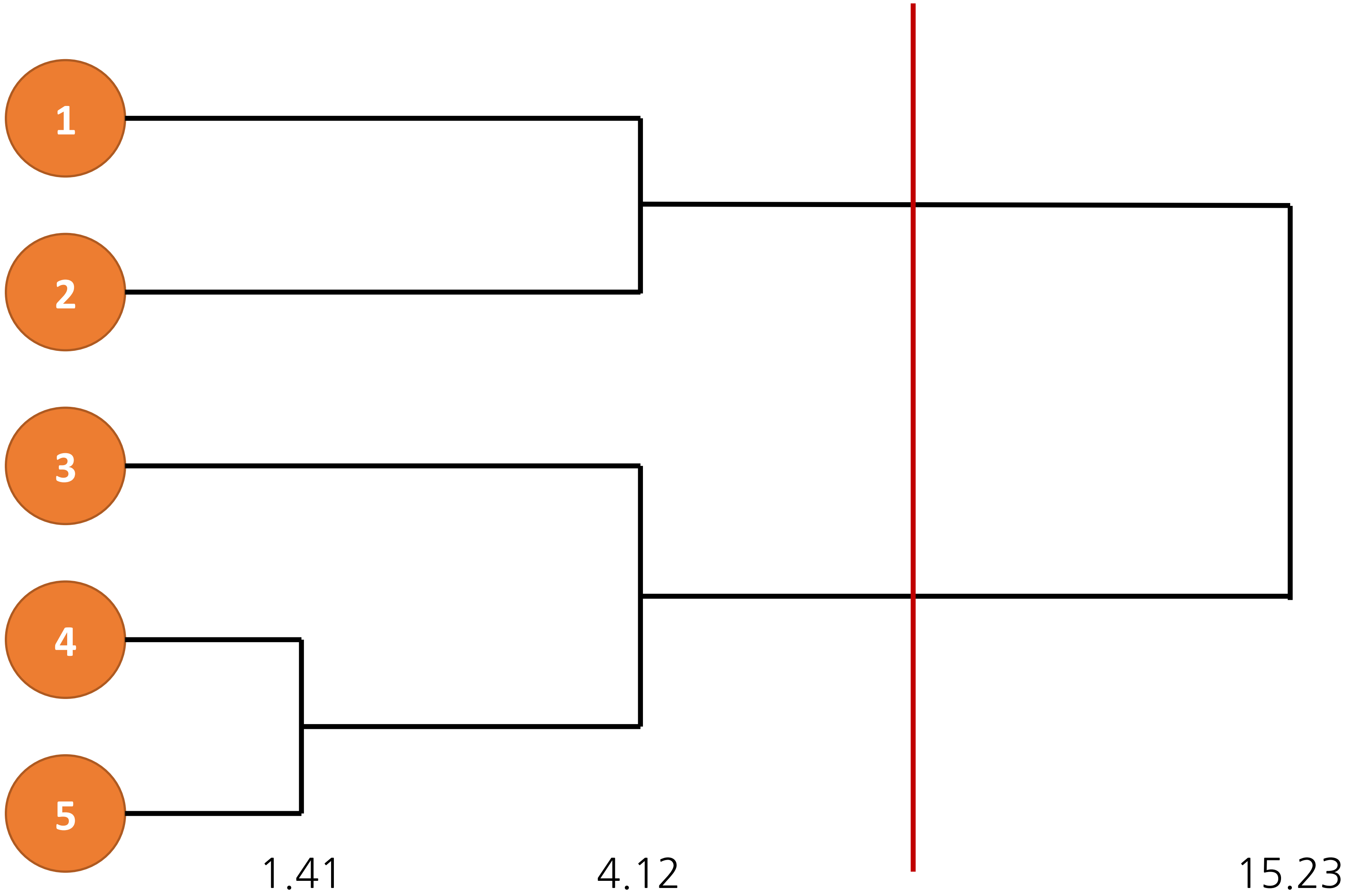
Distance $d(A,B) = \max\{d(a,b): a \in A, b \in B\}$

	7	8
7	0	
8	15.23	0



Example: Complete Linkage Clustering

- **Dendrogram**



Divisive Clustering - DIANA

- **Divisive method starts with one cluster including all samples**
  - At each step, divide cluster into two sub clusters until every cluster consists of one data point
  - This algorithm is based on the average distance between one object and the others

$$\bar{d}(i,C) = \begin{cases} \dfrac{1}{|C|-1} \displaystyle\sum_{j \in C, j \neq i} d(i,j), & if\ i \in C \\ \dfrac{1}{|C|} \displaystyle\sum_{j \in C} d(i,j), & if\ \ i \notin C \end{cases}$$

✓ i represent i-th object

DIANA Algorithm

1
- Consider all samples as one cluster

2
- Select the cluster C containing two objects with the longest distance

3
- Divide cluster C into two as follows (At first, C' is empty set(ϕ))
  - Find object i with maximum $\bar{d}(i, C)$
  - $C \leftarrow C - \{i\}, C' \leftarrow C' \cup \{i\}$
  - If there exist the objects j in C whose $e(j) = \bar{d}(j, C) - \bar{d}(j, C') > 0$, select one of them with maximum $e(j)$, remove j from C and add j into C'
  - If $e(j) < 0$ for all objects in C, finish this step

4
- Repeat step 2 and 3 until the number of clusters is the same as the number of samples

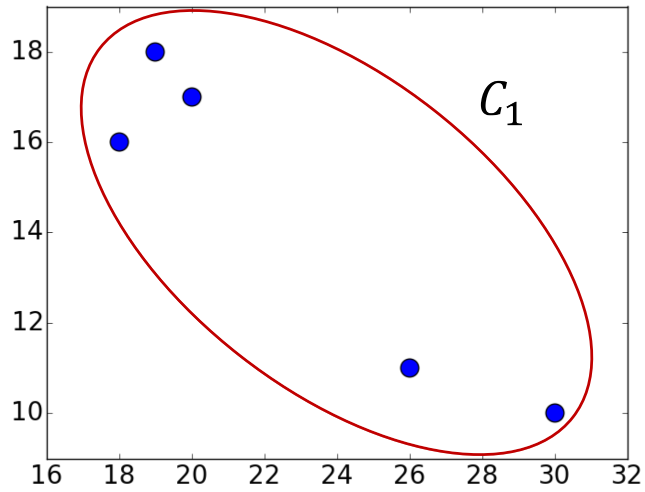
Example: DIANA

- **Find clusters through DIANA**
  - Start with a cluster consisting of all objects
  - $C_1 = \{1,2,3,4,5\}$
  - $C_2 = \{\,\}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 2: Find pair of objects with the longest distance

$d(i,j)$	1	2	3	4	5
1	0				
2	4.12	0			
3	**15.23**	11.18	0		
4	12.21	8.48	4.12	0	
5	13.60	9.90	3.61	1.41	0



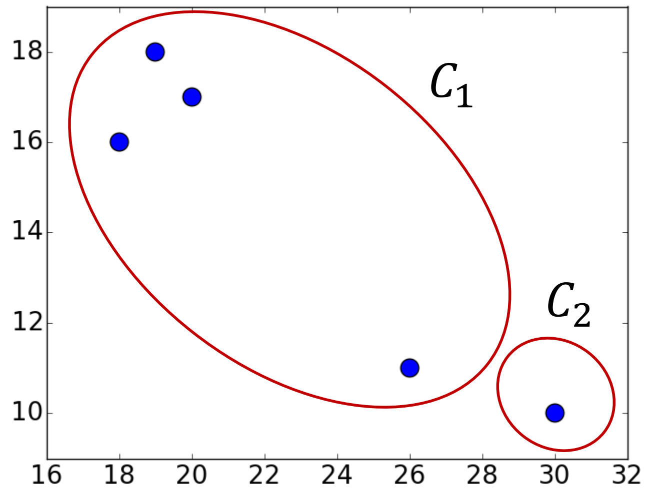
Example: DIANA

- **Find clusters through DIANA**
  - C_1 is the selected cluster

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 3 Find the objects j in C whose $e(j) = \bar{d}(j, C) - \bar{d}(j, C') > 0$

$d(i,j)$	1	2	3	4	5
1	0				
2	4.12	0			
3	15.23	11.18	0		
4	12.21	8.48	4.12	0	
5	13.60	9.90	3.61	1.41	0



↓ Average except 0

	1	2	3	4	5
$\bar{d}\ (i, C_1)$	**11.29**	8.42	8.54	6.56	7.13

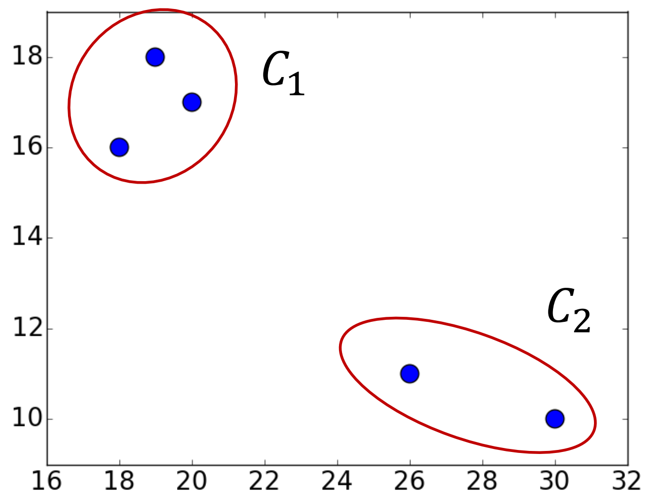
Example: DIANA

- **Find clusters through DIANA**
  - $C_1 = \{2,3,4,5\}, C_2 = \{1\}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 3

	2	3	4	5
$\bar{d}\,(i, C_1)$	9.85	6.30	4.67	4.97
$\bar{d}\,(i, C_2)$	4.12	15.2	12.2	13.6
$e(i)$	**5.73**	-8.9	-7.53	-8.63



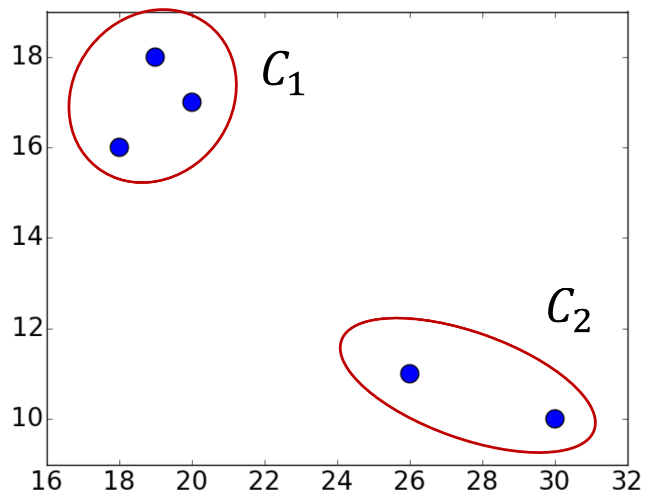
Example: DIANA

- **Find clusters through DIANA**
  - $C_1 = \{3,4,5\}, C_2 = \{1,2\}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 3

	3	4	5
$\bar{d}\,(i, C_1)$	3.87	2.77	2.51
$\bar{d}\,(i, C_2)$	13.21	10.35	11.75
$e(i)$	-9.34	-7.58	-9.24



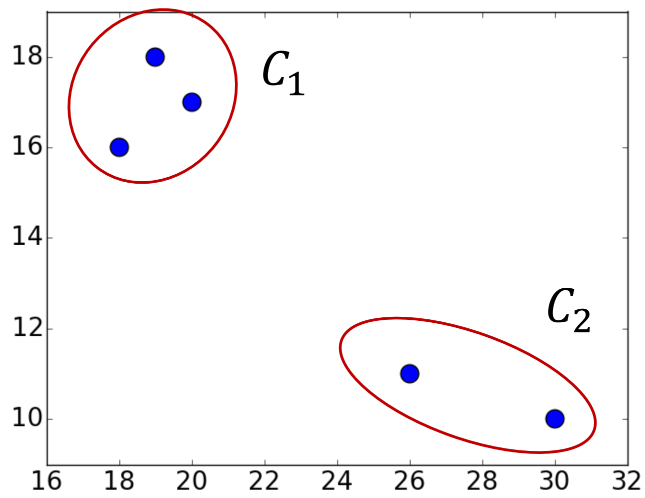
Example: DIANA

- **Find clusters through DIANA**
  - $C_1 = \{3,4,5\}, C_2 = \{1,2\}$
  - Find pair of objects wit the longest distance

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 2: Find pair of objects with the longest distance

$d(i,j)$	1	2	3	4	5
1	0				
2	**4.12**	0			
3			0		
4			**4.12**	0	
5			3.61	1.41	0



Example: DIANA

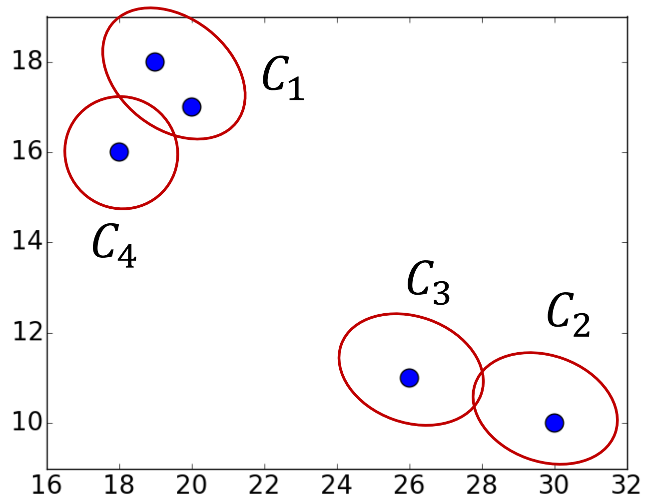
- **Find clusters through DIANA**
  - Select C_2
  - $C_1 = \{1,2\}, C_3 = \{\ \}$
  - C_2 contains only two object, so divide C_2 into two clusters directly: $C_2 = \{1\}, C_3 = \{2\}$

  - Select C_1
  - $C_1 = \{3,4,5\}, C_4 = \{\ \}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 3

	3	4	5
$\bar{d}(i, C_1)$	**3.87**	2.77	2.51



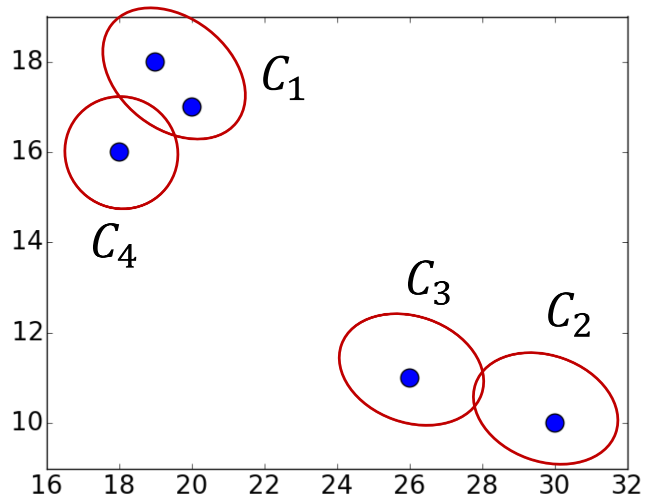
Example: DIANA

- **Find clusters through DIANA**
  - $C_1 = \{4,5\}, C_4 = \{3\}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

Step 3

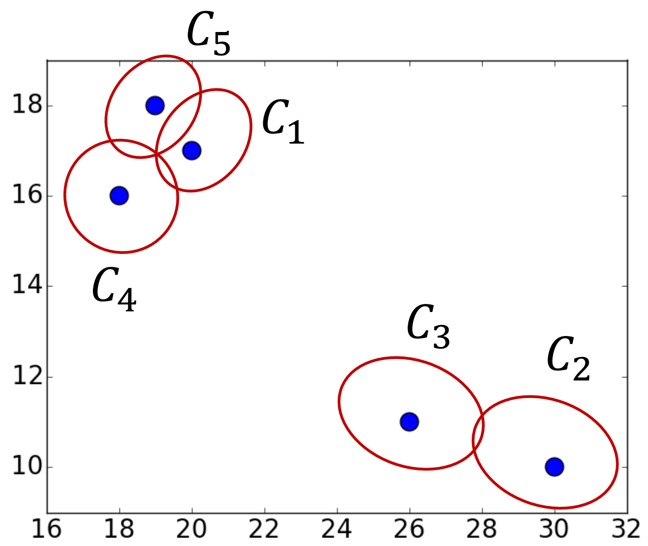
	4	5
$\bar{d}\ (i, C_1)$	1.41	1.41
$\bar{d}\ (i, C_4)$	4.12	3.61
$e(i)$	-2.71	-2.20



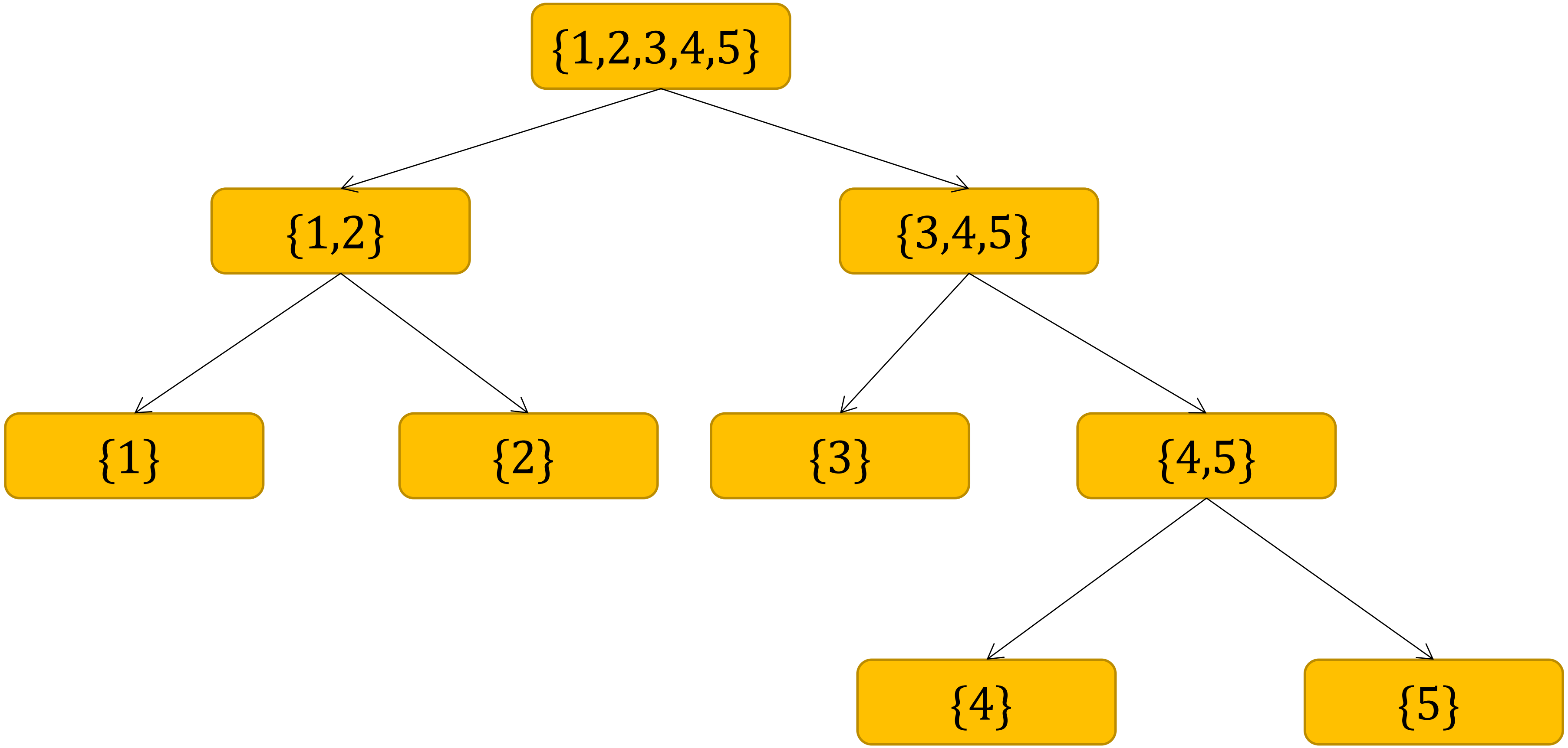
Example: DIANA

- **Find clusters through DIANA**
  - Select C_1
  - $C_1 = \{4,5\}, C_5 = \{\ \}$
  - C_1 contains only two object, so divide C_1 into two clusters directly: $C_1 = \{4\}, C_5 = \{5\}$

	1	2	3	4	5
x	30	26	16	20	19
y	10	11	16	17	18

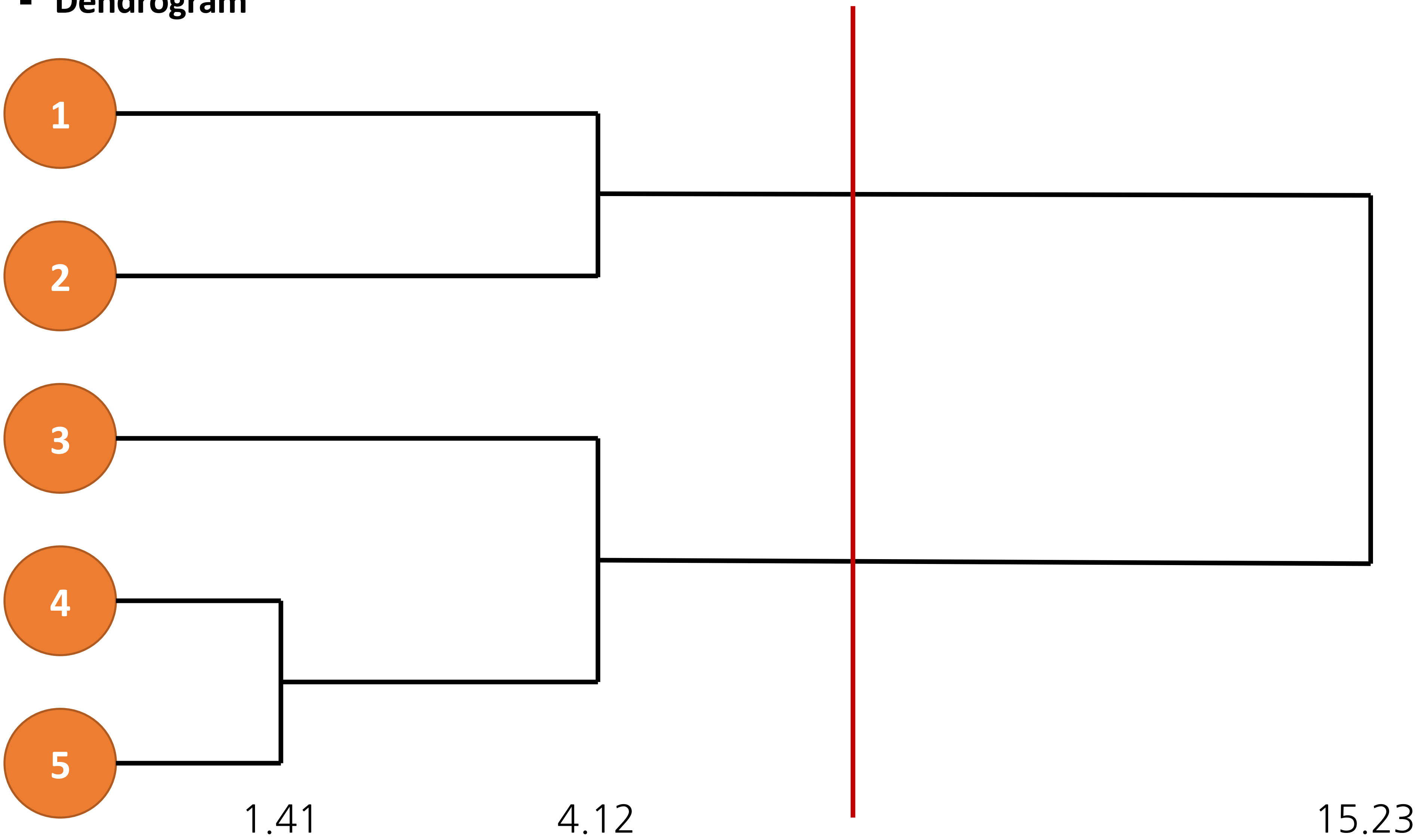


Example: DIANA



Example: DIANA

- **Dendrogram**



Hierarchical Clustering

k-Means Clustering

k-means Clustering

- **Objective function of clustering**

$$\sum_i \min_j \left\| \mathbf{x}_i - \boldsymbol{\mu}_j \right\|^2$$

  - $j \in [1,2,\ldots,k]$
  - $\boldsymbol{\mu}_j$ is the centroid of j-th cluster

⬇

Combinatorial Optimization Problem

k-means Clustering

- **Procedure of k-means clustering**

1
- Set initial k centroids

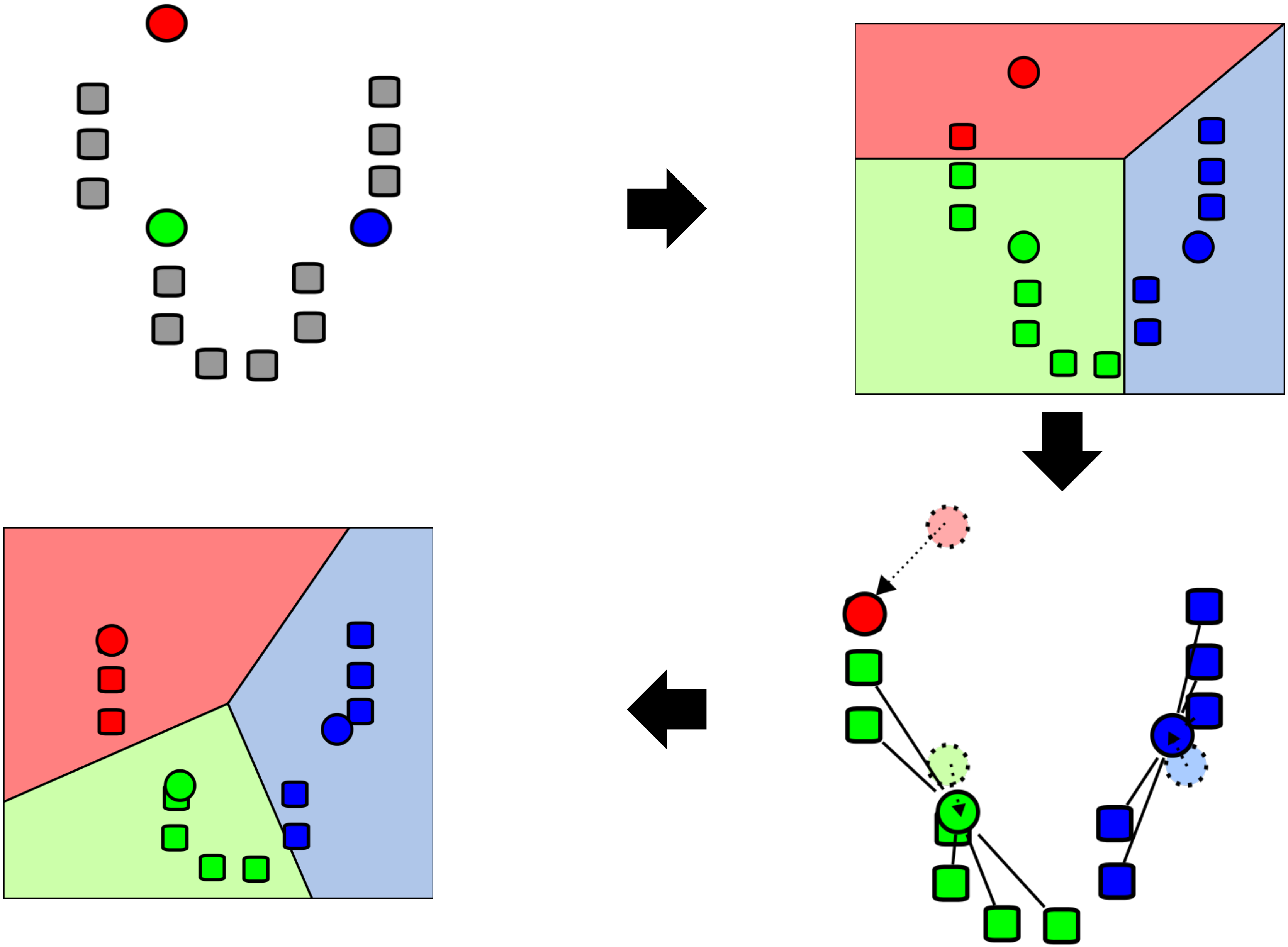
2
- Assign each data point to i-th group whose centroid is the closest to data point among all centroids

3
- Update centroids

4
- Check terminal condition and if condition is not fulfilled, go to step 2

Terminal conditions
[No change in centroids or the number of iteration is over the pre-specified threshold]

k-means Clustering



k-means Clustering

▪ Arithmetic mean

$$m_i^{(t+1)} = \frac{1}{\left|S_i^{(t)}\right|} \sum_{x_j \in S_i^{(t)}} x_j$$

- t is iteration
- m_i is i-th group centroid
- S_i is a set of i-th group and $|S_i|$ is size of S_i

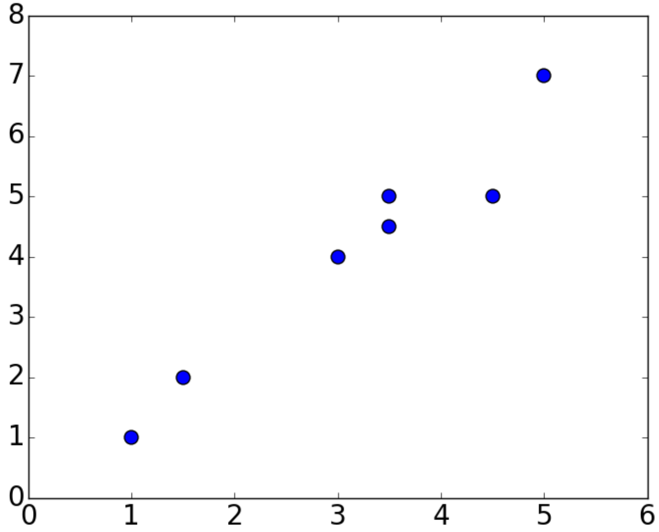
▪ Example

- If (3,1), (2,2), (4,6) belong to group, updated centroid is

$$\left(\frac{3+2+4}{3}, \frac{1+2+6}{3}\right) = (3, 2)$$

Question

- **Clustering for 2D data set**



	1	2	3	4	5	6	7
x	1.0	1.5	3.0	5.0	3.5	4.5	3.5
y	1.0	2.0	4.0	7.0	5.0	5.0	4.5

1) When $k = 2$ and initial centroids are (1.0, 1.0) and (5.0, 7.0), determine group of each data point

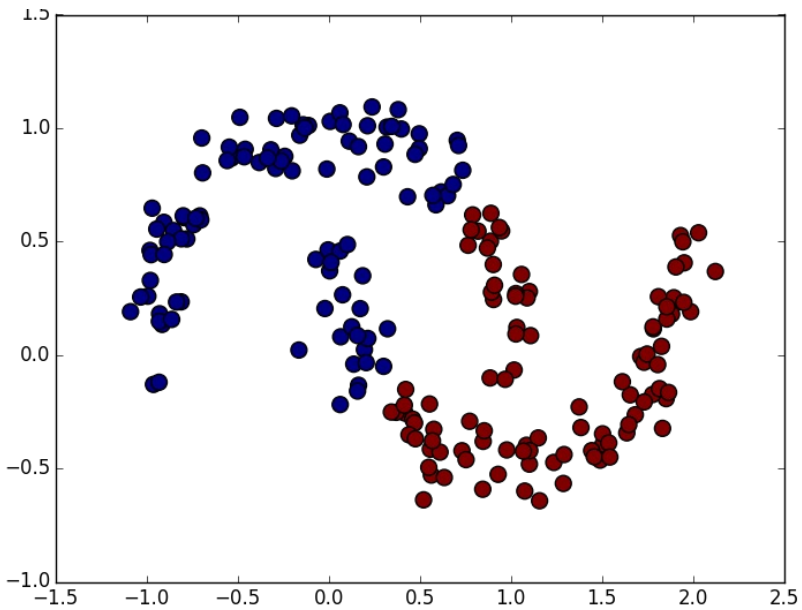
2) What are new centroids of two groups?

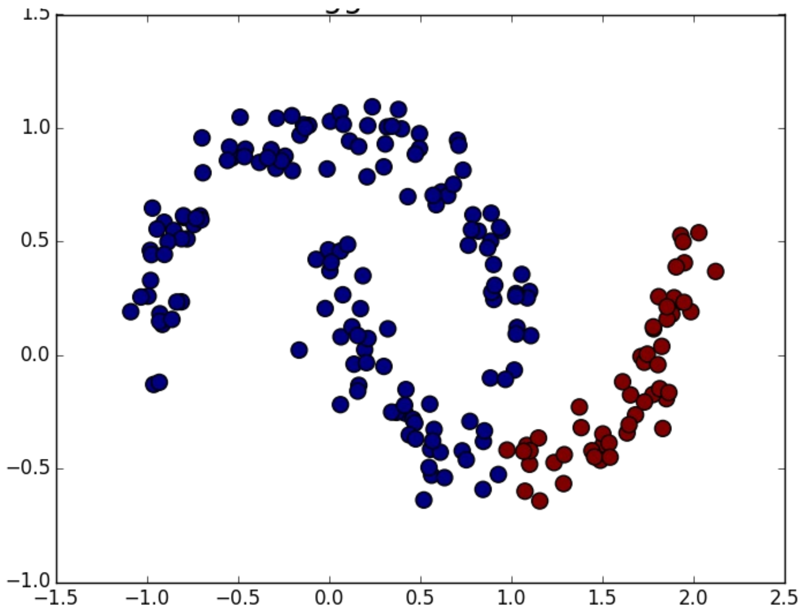
Evaluation Metrics

How to Measure Clustering Quality

- **Clustering problem is unsupervised problem**
  - No explicit answer for learning
  - We need to define a method to measure quality of clustering

Which one is better?





How to Measure Clustering Quality

- **Measures that do not require ground truth labels**
  - Inertia
    - ✓ Within-cluster sum-of-squares

$$\sum_{i=0}^{n} \min_{\mu_j \in C} \left\| x_j - \mu_i \right\|^2$$

  - Silhouette Coefficient
    - ✓ $s(i)$: Silhouette coefficient of i-th sample
    - ✓ $a(i)$: The mean distance between a sample and all other points in the same class
    - ✓ $b(i)$: The mean distance between a sample and all other points in the next nearest cluster

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

$$-1 \leq s(i) \leq 1$$

    - ✓ Overall clustering quality can be obtained by averaging $s(i)$ for all samples

How to Measure Clustering Quality

- **Clustering performance evaluation measure**
  - Homogeneity: each cluster contains only members of a single class

$$h = 1 - \frac{H(C|K)}{H(C)}$$

  ✓ $H(C)$ is the entropy of the classes

$$H(C) = -\sum_{c=1}^{|C|} \frac{n_c}{n} \cdot \log\left(\frac{n_c}{n}\right)$$

  ✓ $H(C|K)$ is the conditional entropy of the classes given the cluster assignments

$$H(C|K) = -\sum_{c=1}^{|C|} \sum_{k=1}^{|K|} \frac{n_{c,k}}{n} \log\left(\frac{n_{c,k}}{n_k}\right)$$

  ✓ n is the total number of samples, n_c and n_k are the number of samples respectively belonging to class c and cluster k

  ✓ $n_{c,k}$ is the number of samples from class c assigned to cluster k

  - Completeness: all members of a given class are assigned to the same cluster

$$c = 1 - \frac{H(K|C)}{H(K)}$$

How to Measure Clustering Quality

- **Contingency table**

$$\binom{n}{k} = {}_nC_k$$

	K_1	K_2	$\cdots$	K_s	$sums$
C_1	n_{11}	n_{12}	$\cdots$	n_{1s}	a_1
C_2	n_{21}	n_{22}	$\cdots$	n_{2s}	a_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
C_r	n_{r1}	n_{r2}	$\cdots$	n_{rs}	a_r
$sums$	b_1	b_2	$\cdots$	b_s	n

- a is the number of pairs, elements of which are in the same class and in the same cluster.
  - ✓ a_{ij} is the number of pairs that belong to a and can be counted by selecting two samples among n_{ij} samples.
  - ✓ $a = \sum_{ij} a_{ij} = \sum_{ij} \binom{n_{ij}}{2}$
- b is the number of pairs, elements of which are in different classes and in different clusters.
  - ✓ b can be calculated by subtracting $(a + b + c)$ from the number of all pairs $\binom{n}{2}$
- c is the number of pairs, elements of which are in the same class and in different clusters.
  - ✓ $c = \sum_i c_i$ where c_i is the number of pairs in c for the class i.
  - ✓ c_i can be calculated by subtracting the number of pairs in the same class and cluster $\sum_j \binom{n_{ij}}{2}$from the number of pairs in same class pairs $\binom{a_i}{2}$
  - ✓ $c = \sum_i \binom{a_i}{2} - \sum_{ij} \binom{n_{ij}}{2}$
- d is the number of pairs, elements of which are in different classes and in the same clusters.
  - ✓ $d = \sum_j \binom{b_j}{2} - \sum_{ij} \binom{n_{ij}}{2}$ can be calculated in the similar way.

How to Measure Clustering Quality

- **Rand index (RI)**
  - RI is the ratio of corrected distributed pairs.
  - As we saw in the previous page, we can categorize each pair of data samples into four categories.
  - Rand index measures the ratio of pairs located in the same class and cluster or in different classes and clusters among all pairs.
  - According to our definition in the previous page, we can define $RI = \frac{a+b}{a+b+c+d}$

How to Measure Clustering Quality

- **Clustering performance evaluation measure**
  - Limitation of RI
    - ✓ As the number of clusters increases, the probability that two data samples are in different clusters increases. This trend leads to biased result (i.e., RI will increase as the number of cluster increases.)
  - Adjusted Rand Index(ARI)
    - ✓ Given the knowledge of the ground truth class assignments and our clustering algorithm assignments of the same samples, the adjusted Rand index is a function that measures the similarity of the two assignments

$$\mathrm{ARI} = \frac{\mathrm{RI} - \mathbb{E}[\mathrm{RI}]}{\max(\mathrm{RI}) - \mathbb{E}[\mathrm{RI}]}$$

    - ✓ C is a ground truth class assignment, K is the clustering
    - ✓ a is the number of pairs of elements that are in the same set in C and in the same set in K
    - ✓ b is the number of pairs of elements that are in different sets in C and in different sets in K
    - ✓ Raw Rand index $\mathrm{RI} = \frac{a+b}{C_2^n}$($C_2^n$ is the total number of possible pairs in the dataset)

$$C_2^n = \frac{n!}{2!\,(n-2)!}$$

How to Measure Clustering Quality

- **Contingency table**

	K_1	K_2	$\cdots$	K_s	$sums$
C_1	n_{11}	n_{12}	$\cdots$	n_{1s}	a_1
C_2	n_{21}	n_{22}	$\cdots$	n_{2s}	a_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
C_r	n_{r1}	n_{r2}	$\cdots$	n_{rs}	a_r
$sums$	b_1	b_2	$\cdots$	b_s	n

$$\mathrm{ARI} = \frac{\mathrm{RI} - \mathbb{E}[\mathrm{RI}]}{\max(\mathrm{RI}) - \mathbb{E}[\mathrm{RI}]} = \frac{\sum_{ij}\binom{n_{ij}}{2} - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}\right] - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}$$

Hubert, L., Arabie, P. Comparing partitions. *Journal of Classification* **2**, 193–218 (1985). https://doi.org/10.1007/BF01908075

$$\binom{n}{k} = {}_nC_k$$

How to Measure Clustering Quality

- **[Drawbacks]**
  Homogeneity, Completeness, and ARI require knowledge of the ground truth classes while is almost never available in practice or require manual assignment by human annotators

Thank you!