

Data Clustering

Danushka Bollegala



Outline

- Why cluster data?
- Clustering as unsupervised learning
- Clustering algorithms
 - **k-means**, k-medoids
 - **agglomerative clustering**
 - Brown's clustering
 - Spectral clustering
- Cluster evaluation measures
 - **Purity**
 - **Normalised Mutual Information**
 - **Rand Index**
 - **B-CUBED**
 - **Precision, Recall, F-score**
- Supervised clustering

We look only at topics shown in red here

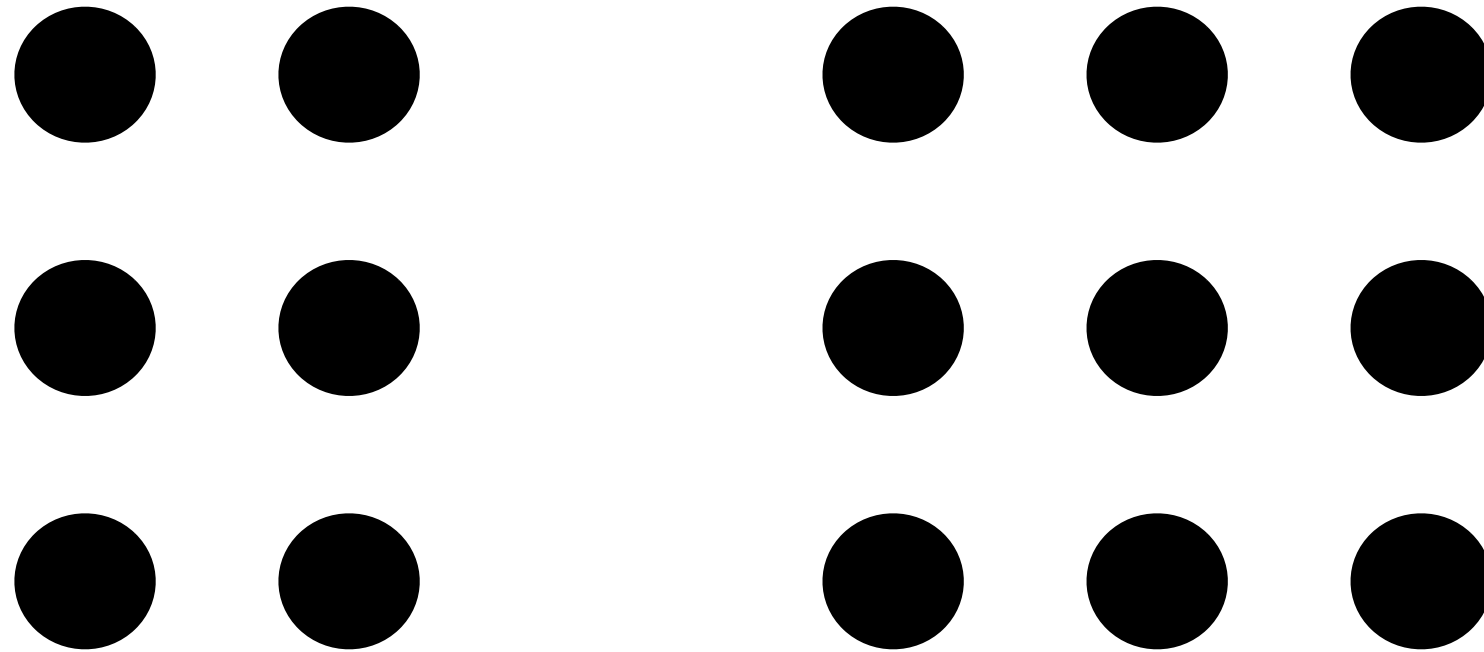
Why cluster data?

- Data Mining has two main objectives
 - Prediction: classification, regression etc.
 - Description: pattern mining, rule extraction, visualisation *clustering*
- Clustering is:
 - Unsupervised learning
 - no label data is required (consider classification algorithms we discussed so far in the lecture which are supervised algorithms)
 - Generalisation / Abstraction of concepts
 - Topic detection
 - Visualisation
 - Outlier detection

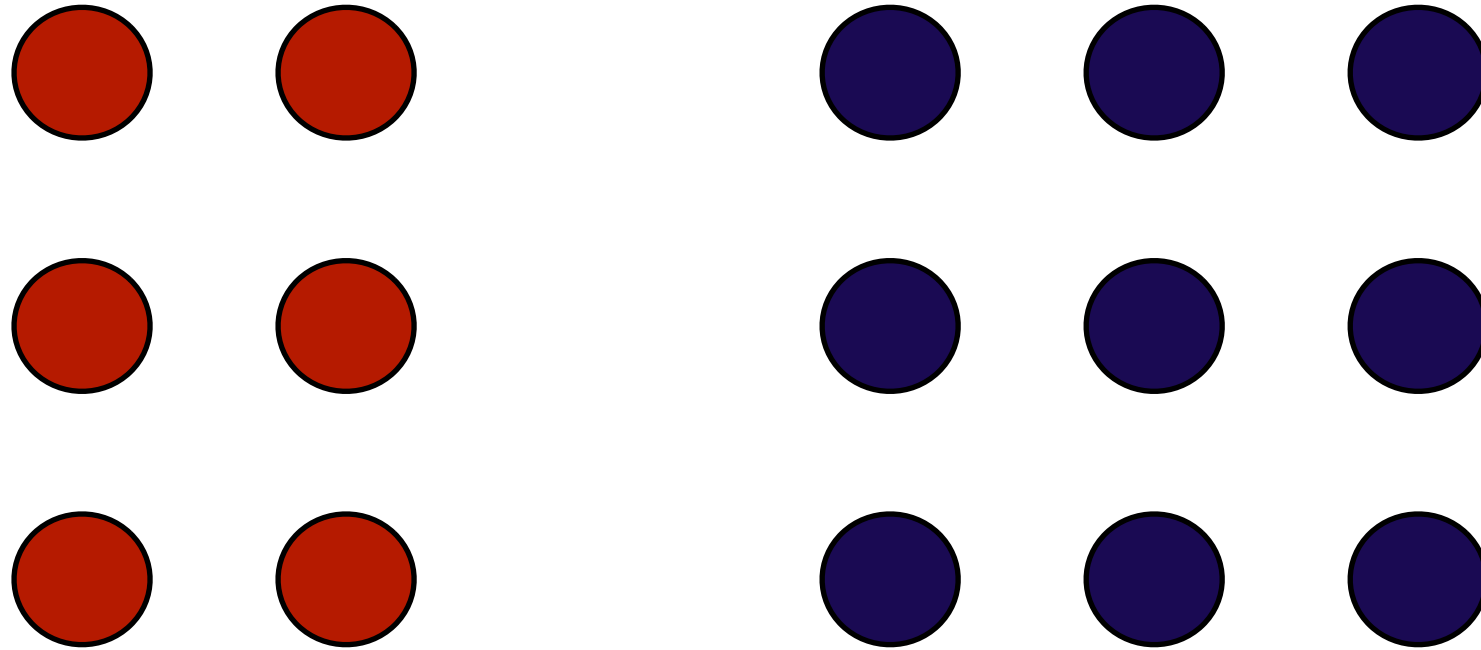
Unsupervised Learning

- Supervised learning
 - labels for training instances are provided
- Unsupervised learning
 - No labels for training instances are provide
- Semi-supervised learning
 - Both labeled and unlabeled training instances are provided
- What can we learn about training data if we do not have any labels?
 - The similarity and distribution of the features can still be learnt and this can be used to create rich feature spaces for supervised learning (if required)

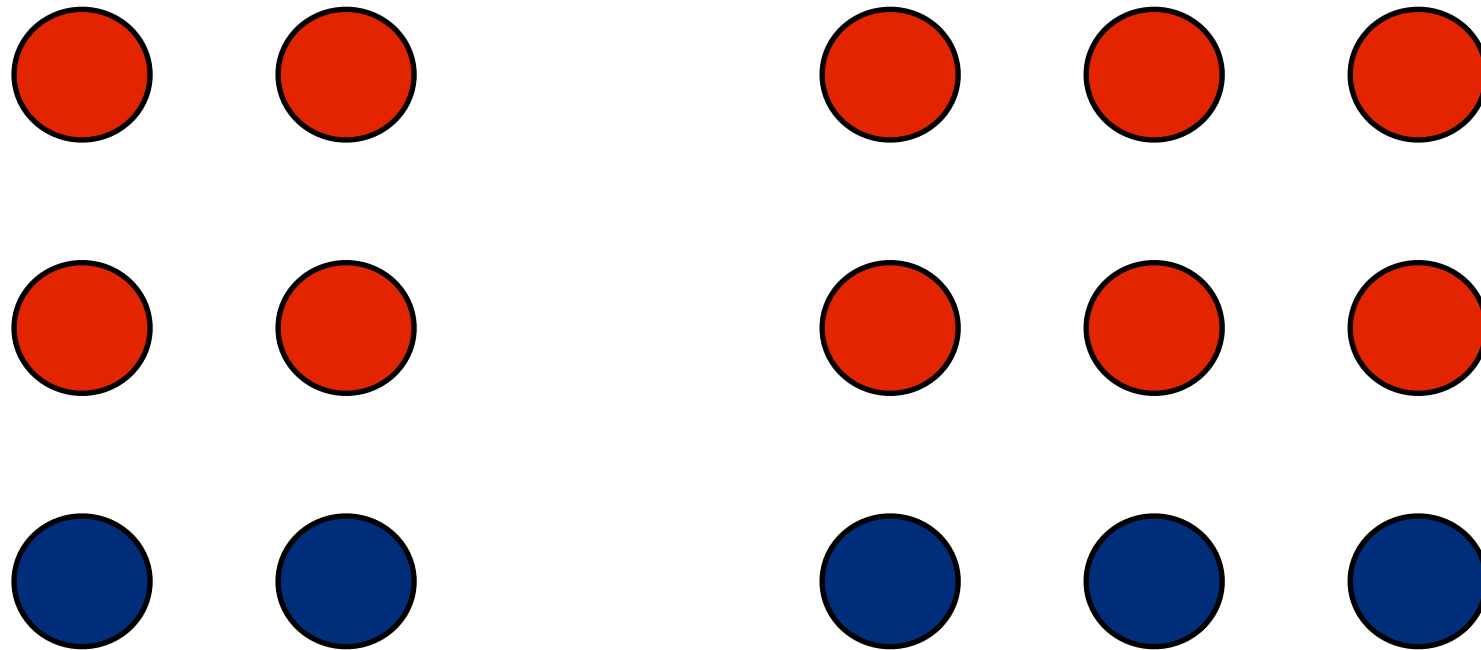
Quiz: Cluster the Following Data



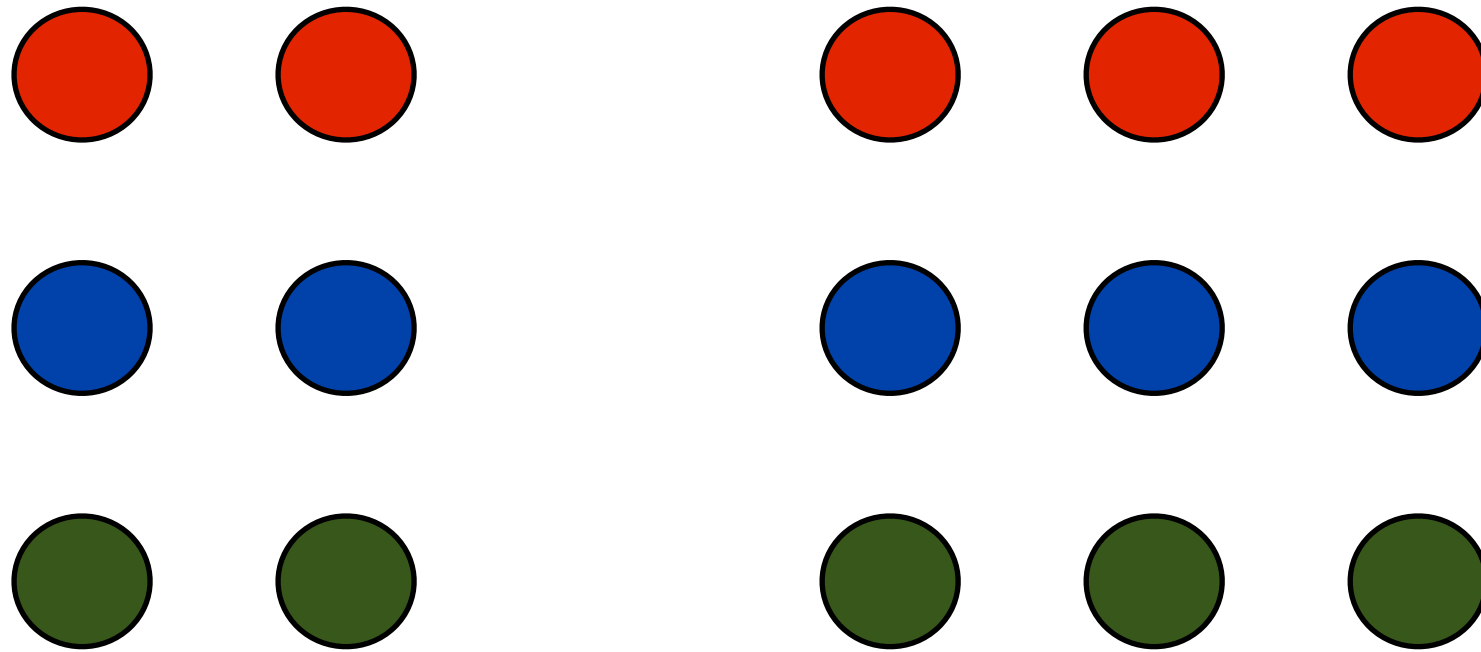
Quiz: Cluster the Following Data



Quiz: Cluster the Following Data



Quiz: Cluster the Following Data



How many clusters?

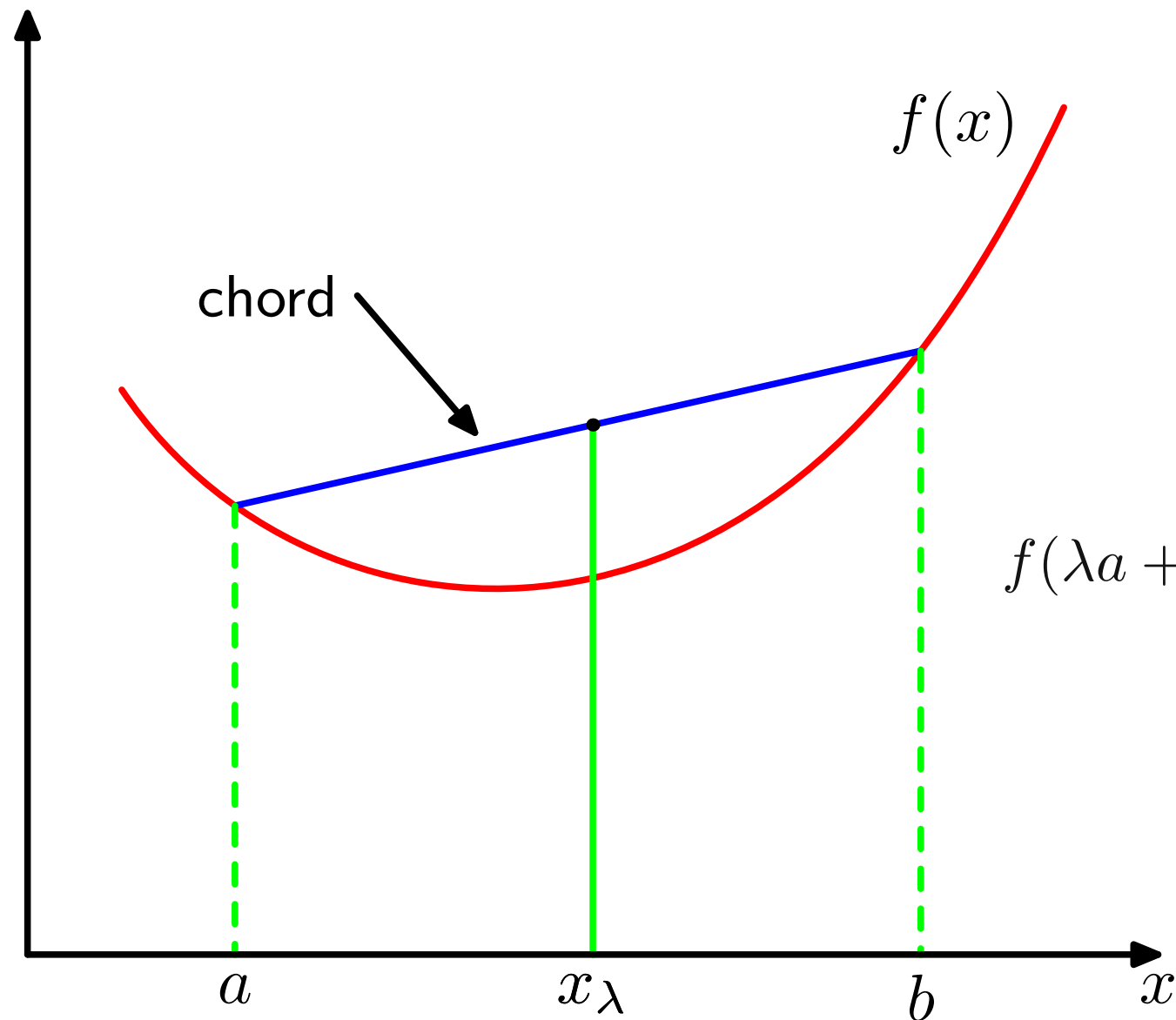
General Remarks

- A single dataset can be clustered into several ways
- There is no single right or wrong clustering
 - Simply different views on the same data
- If so how can we measure the quality of a clustering algorithm?
 - Two ways
 - Compare the clusters produced by a clustering algorithm against some reference (gold standard) set of clusters (**direct evaluation**)
 - Use the clusters as features for some other (eg. supervised learning) task and measure the difference in the performance of the second task (**indirect evaluation**)

Clustering as Optimisation

- Given a dataset $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of N instances represented as d dimensional real vectors ($\mathbf{x}_i \in \mathbb{R}^d$), partition these N instances into k clusters S_1, \dots, S_k such that some objective function $f(S_1, \dots, S_k)$ is minimised.
- Observations
 - k and f are given
 - f can be the similarity between the clusters (good to create dissimilar clusters as much as possible), information gain, correlation and various other such *goodness* measures (heuristics)
 - Often clustering is an NP hard and a non-convex problem
 - <http://rangevoting.org/VattaniKmeansNPC.pdf>
 - approximations, relaxations are required in practice

Convex Functions



$$f(\lambda a + (1 - \lambda)b) \leq \lambda f(a) + (1 - \lambda)f(b).$$

Clustering Algorithms

- Partitioning
 - Construct k partitions and iteratively update the partitions
 - k-Means, k-Medoids
- Hierarchical
 - Create a hierarchy of clusters (dendrogram)
 - Agglomerative clustering (bottom-up)
 - Conglomerative clustering (top-down)
- Graph-based clustering
 - Graph-cut algorithms (Spectral Clustering)
- Model-based clustering
 - Mixture of Gaussians
- Other types: Non-parametric Bayesian (Latent Dirichlet Allocation), Expectation Maximisation (EM) algorithm, and many more ...

k-Means Derivation

$$\arg \min_{S_1, \dots, S_k} \sum_{i=1}^k \sum_{\mathbf{x}_j \in S_i} \|\mathbf{x}_j - \boldsymbol{\mu}_i\|^2$$

We want to minimize the distance between data instances (\mathbf{x}_j) and some cluster centres ($\boldsymbol{\mu}_i$)

$$f(S_1, \dots, S_k) = \sum_{i=1}^k \sum_{\mathbf{x}_j \in S_i} \|\mathbf{x}_j - \boldsymbol{\mu}_i\|^2$$

This objective function is called the *within cluster sum of squares* (WCSS) objective

$$\frac{\partial f(S_1, \dots, S_k)}{\partial \mu_i} = 0$$

$$\frac{\partial f(S_1, \dots, S_k)}{\partial \mu_i} = \sum_{\mathbf{x}_j \in S_i} 2(\mathbf{x}_j - \mu_i)$$

$$\mu_i = \frac{1}{|S_i|} \sum_{\mathbf{x}_j \in S_i} \mathbf{x}_j$$

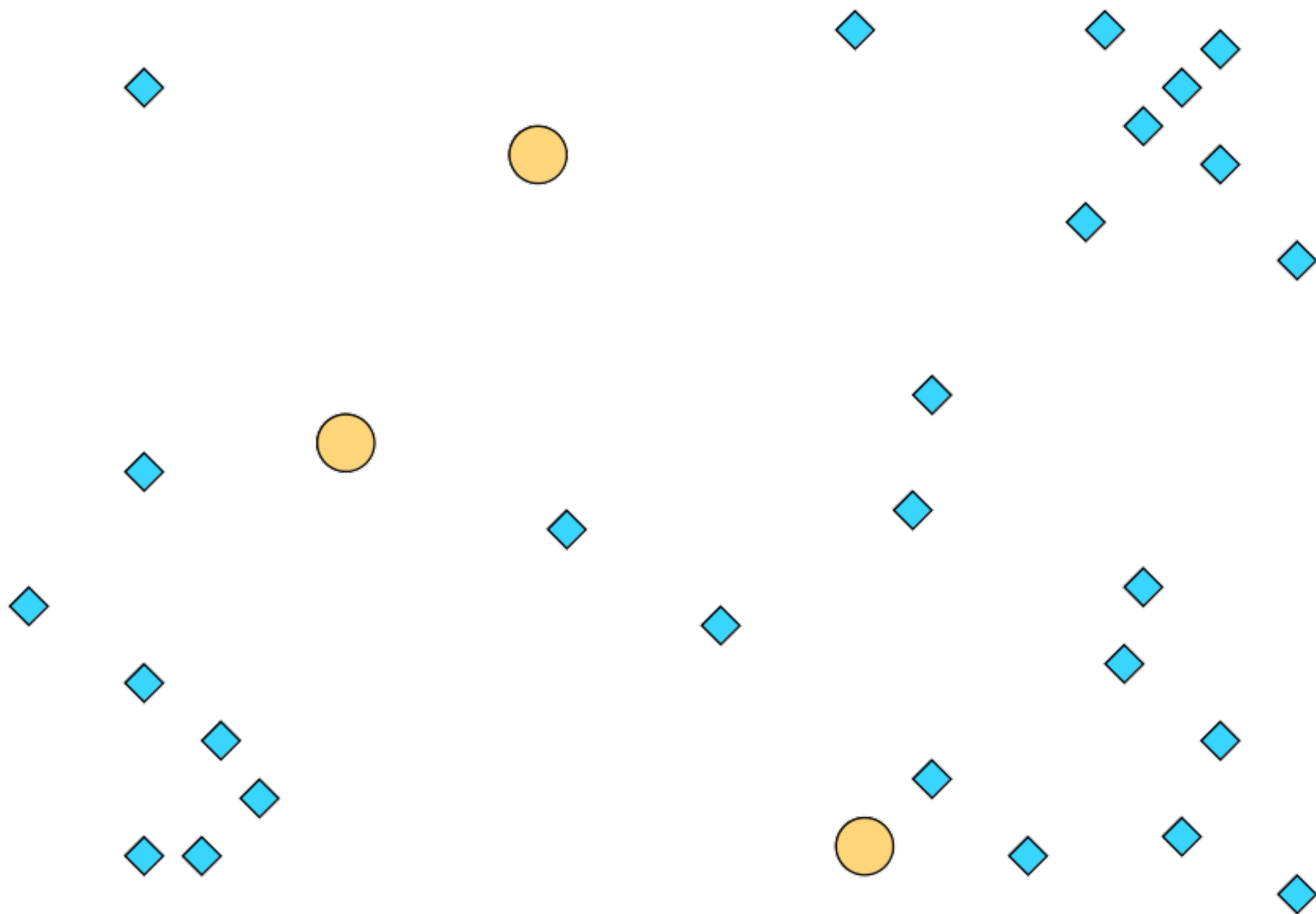
Just compute the centroid (mean) of each cluster and that will give you the cluster centers

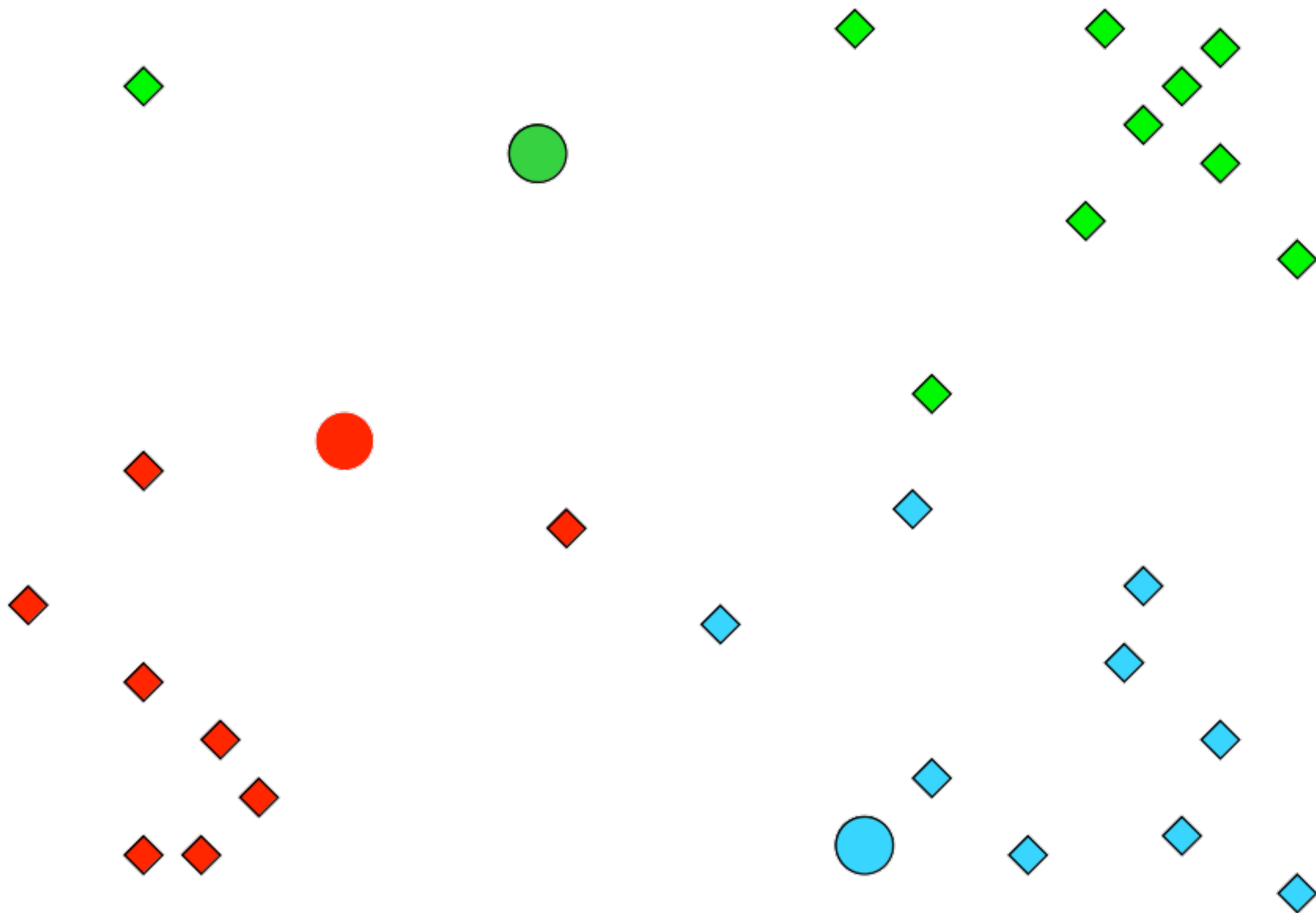
k-Means Clustering

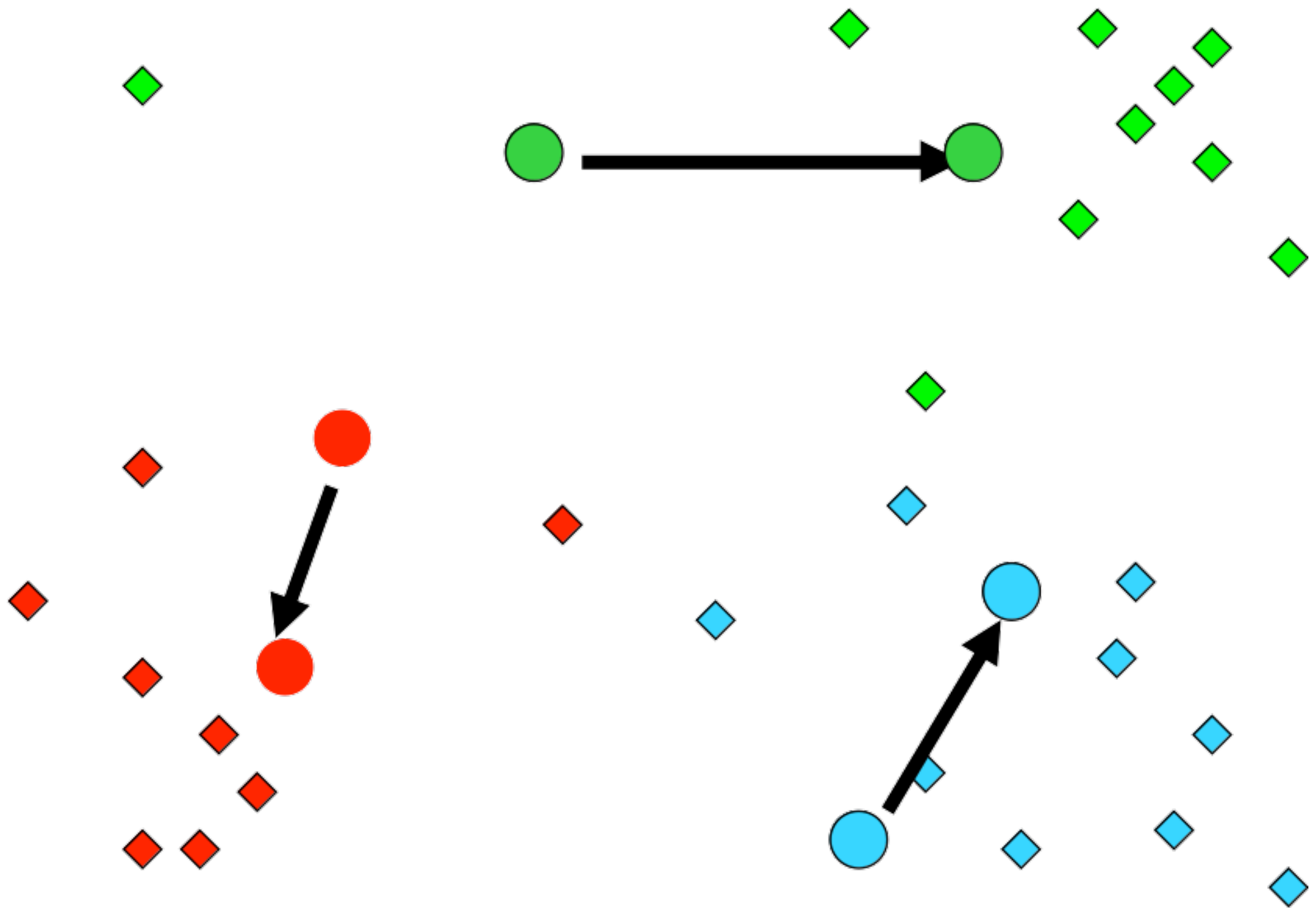
- INPUT

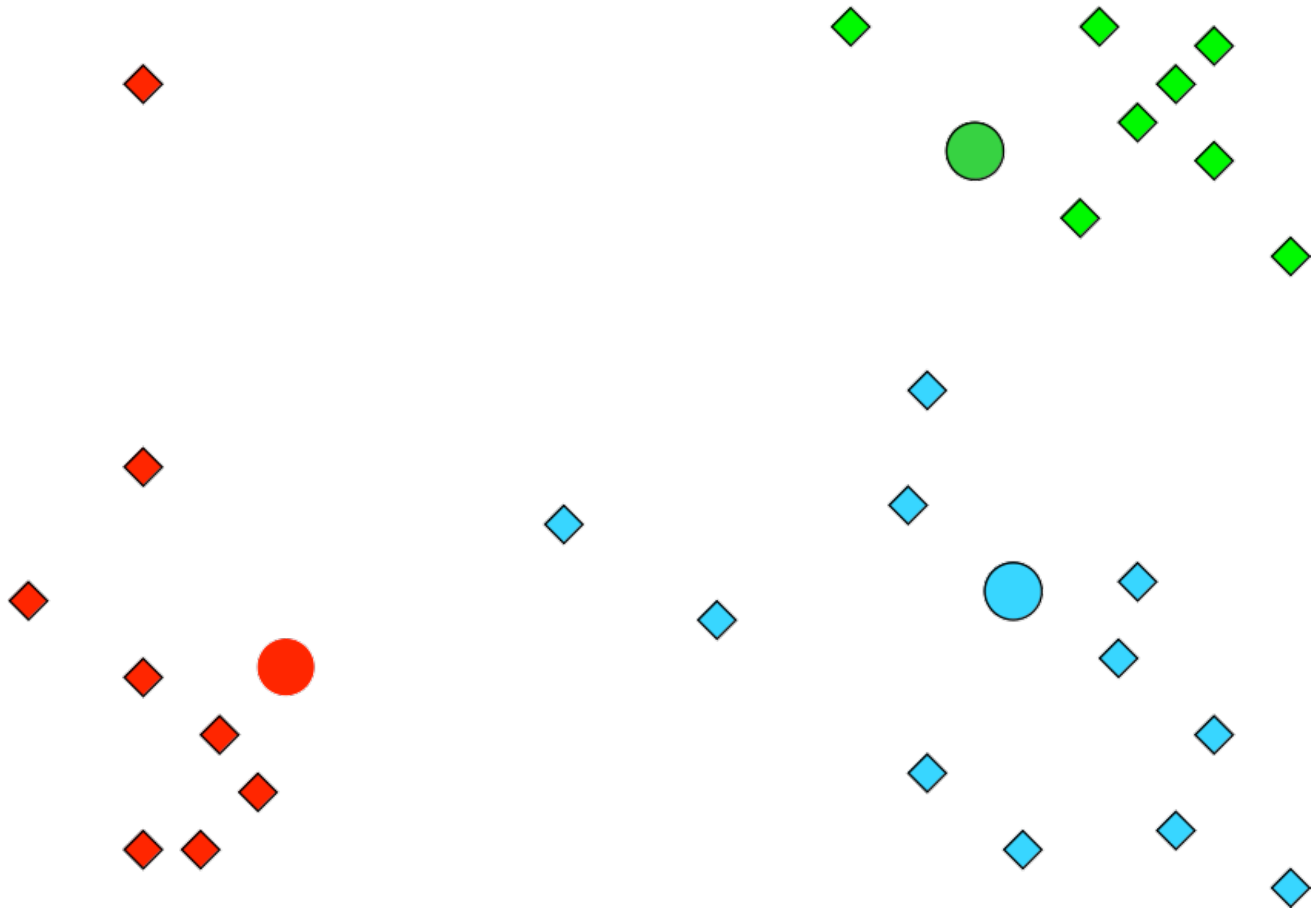
- The number of clusters k
- Dataset $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of N instances represented as d dimensional real vectors ($\mathbf{x}_i \in \mathbb{R}^d$)

1. Set k instances from the dataset randomly. (initial cluster means/centers)
2. Assign all other instances to the closest cluster centre.
3. Compute the mean of each cluster
4. until **convergence** repeat between steps 2 and 3
convergence = no instances have moved among clusters
(often after a fixed number of iterations specified by the user)









Issues with k-Means

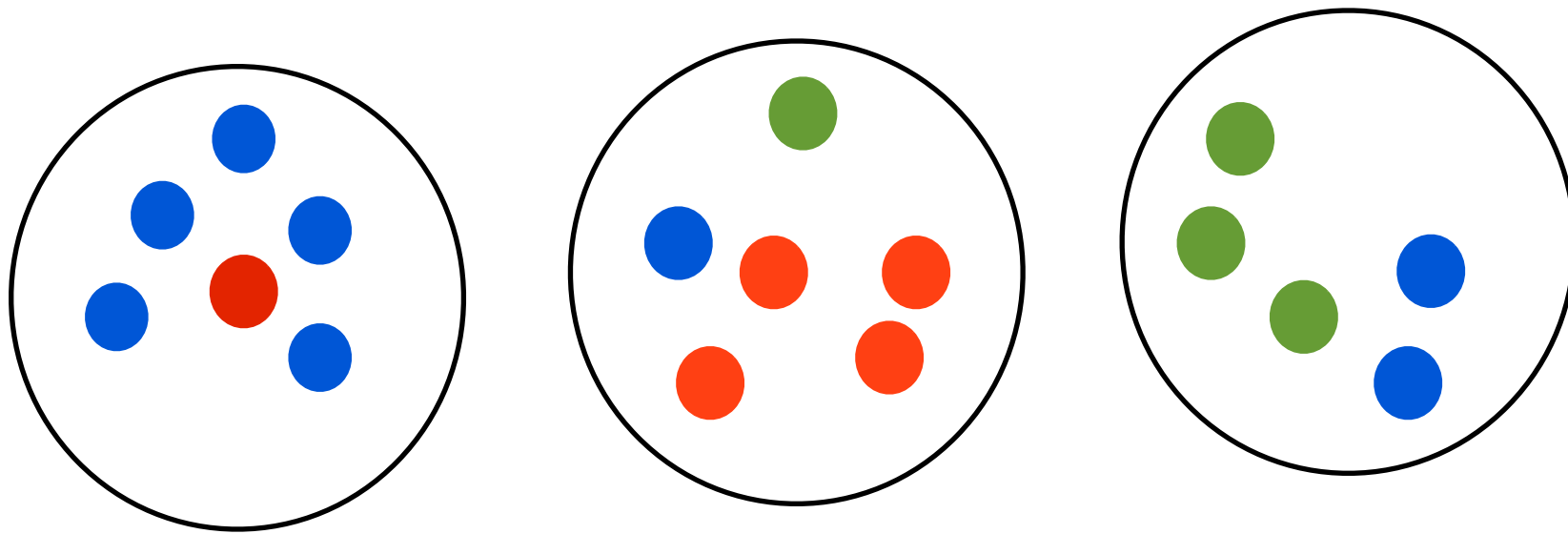
- Results can vary depending on the initial random choices
- Can get trapped in a local minimum that isn't the global optimal solution
 - Repeat the clustering procedure multiple times with different initialisations and select the *best* final clustering
 - *best?* according to what? many heuristics exist.
 - smallest number of iterations before convergence
 - largest total distance between the final cluster means
- Outliers have a larger effect on the mean value, hence cluster centre and the cluster
- cluster centres (means) are not actual instances in the cluster
 - We could pick actual instances as initial cluster centroids.

Evaluating Clustering — Purity

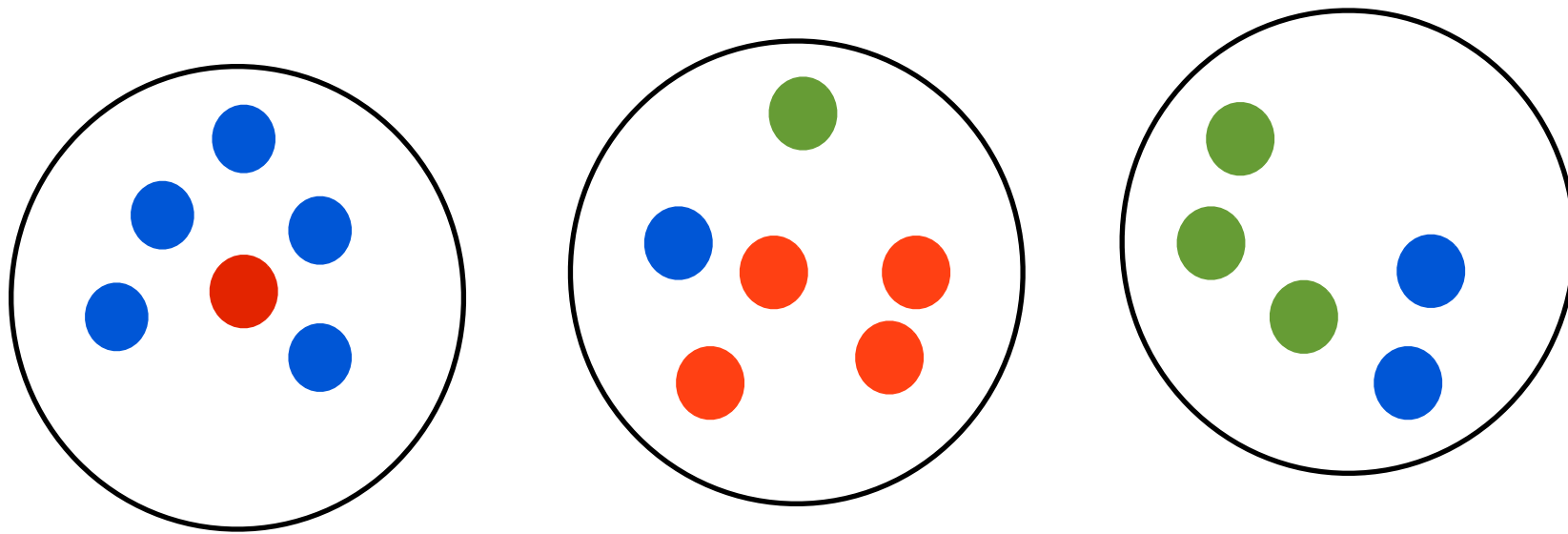
- Let us assume that we have a set $\Omega = \{\omega_1, \dots, \omega_K\}$ clusters for a set of classes $C = \{c_1, \dots, c_J\}$
- Purity measures the ratio of the items that are in the cluster with the same class as its own.

$$\text{purity}(\Omega, C) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j|$$

- Here, N is the total number of items.



Quiz: Compute purity for this clustering.



Labels ●



$$\text{purity} = (5 + 4 + 3) / 17 = 12/17 = 0.71$$

Purity achieves its maximum value of 1 for singletons (each item is in a cluster containing only that single item)! Obviously this is not good “clustering” and purity does not recognise this.

Evaluating Clustering — NMI

- Let us assume that we have a set $\Omega = \{\omega_1, \dots, \omega_K\}$ clusters for a set of classes $\mathcal{C} = \{c_1, \dots, c_J\}$
- Normalised Mutual Information (NMI) computes the ratio of information that we can know about the classes \mathcal{C} given the clusters Ω to the averaged information that is contained in \mathcal{C} and Ω .

$$\text{NMI}(\Omega, \mathcal{C}) = \frac{I(\Omega, \mathcal{C})}{[H(\Omega) + H(\mathcal{C})]/2}$$

$$\begin{aligned} I(\Omega, \mathcal{C}) &= \sum_k \sum_j p(\omega_k \cap c_j) \log \left(\frac{p(\omega_k \cap c_j)}{p(\omega_k)p(c_j)} \right) \\ &= \sum_k \sum_j \frac{|\omega_k \cap c_j|}{N} \log \left(\frac{N|\omega_k \cap c_j|}{|\omega_k||c_j|} \right) \end{aligned}$$

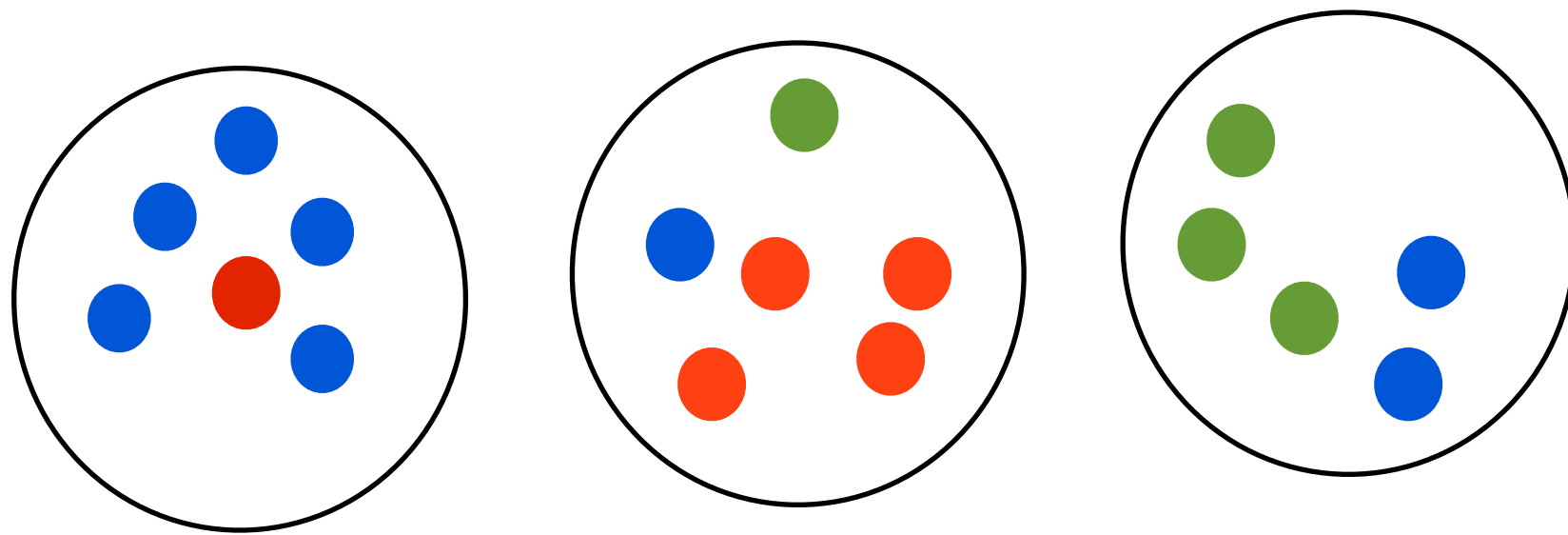
Mutual Information (MI)

$$\begin{aligned} H(\Omega) &= - \sum_k p(\omega_k) \log p(\omega_k) \\ &= - \sum_k \frac{|\omega_k|}{N} \log \frac{|\omega_k|}{N} \end{aligned}$$

Entropy

Why we do we normalise by the average?

- $I(X,Y) \leq [H(X) + H(Y)]/2$
- Proof (sketch):
 - $I(X,Y) = H[X] - H[X|Y] = H[Y] - H[Y|X]$
 - Add those two and use the fact that (conditional) entropy is nonnegative
 - $H[X|Y] + H[Y|X] \geq 0$



Quiz: Compute NMI for this clustering.

Let $C_1 = \text{Blue}$, $C_2 = \text{Red}$ and $C_3 = \text{Green}$.

$$P(C_1) = \frac{8}{17}, \quad P(C_2) = \frac{5}{17}, \quad P(C_3) = \frac{4}{17}.$$

$$\begin{aligned} \therefore H(C) &= - \sum_{i=1}^3 P(C_i) \log P(C_i) \\ &= - \left[\frac{8}{17} \log \frac{8}{17} + \frac{5}{17} \log \frac{5}{17} + \frac{4}{17} \log \frac{4}{17} \right] = 1.055 \end{aligned}$$

Likewise,
 $P(\omega_1) = \frac{6}{17}, \quad P(\omega_2) = \frac{6}{17}, \quad P(\omega_3) = \frac{5}{17}$

$$H(\Omega) = - \left[\frac{6}{17} \log \frac{6}{17} + \frac{6}{17} \log \frac{6}{17} + \frac{5}{17} \log \frac{5}{17} \right] = 1.095$$

$$P(\omega_1 \cap C_1) = \frac{5}{17} \quad P(\omega_1 \cap C_2) = \frac{1}{17} \quad P(\omega_1 \cap C_3) = \frac{0}{17}$$

$$P(\omega_2 \cap C_1) = \frac{1}{17} \quad P(\omega_2 \cap C_2) = \frac{4}{17} \quad P(\omega_2 \cap C_3) = \frac{1}{17}$$

$$P(\omega_3 \cap C_1) = \frac{2}{17} \quad P(\omega_3 \cap C_2) = \frac{0}{17} \quad P(\omega_3 \cap C_3) = \frac{3}{17}$$

$$I(\omega, C) = \sum_{k=1}^2 \sum_{j=1}^3 P(\omega_k \cap C_j) \log \frac{P(\omega_k \cap C_j)}{P(\omega_k) P(C_j)} = 0.4496$$

$$\therefore NMI(\omega, C) = \frac{I(\omega, C)}{(H(\omega) + H(C))/2} = \frac{0.4496}{(1.055 + 1.095)/2} = 0.4182$$

```
import math

C = [5,1,1,4,1,2,3]

p = []
N = sum(C)
for x in C:
    p.append(float(x) / float(N))

E = 0
for x in p:
    E += - x * math.log(x)

print E
```

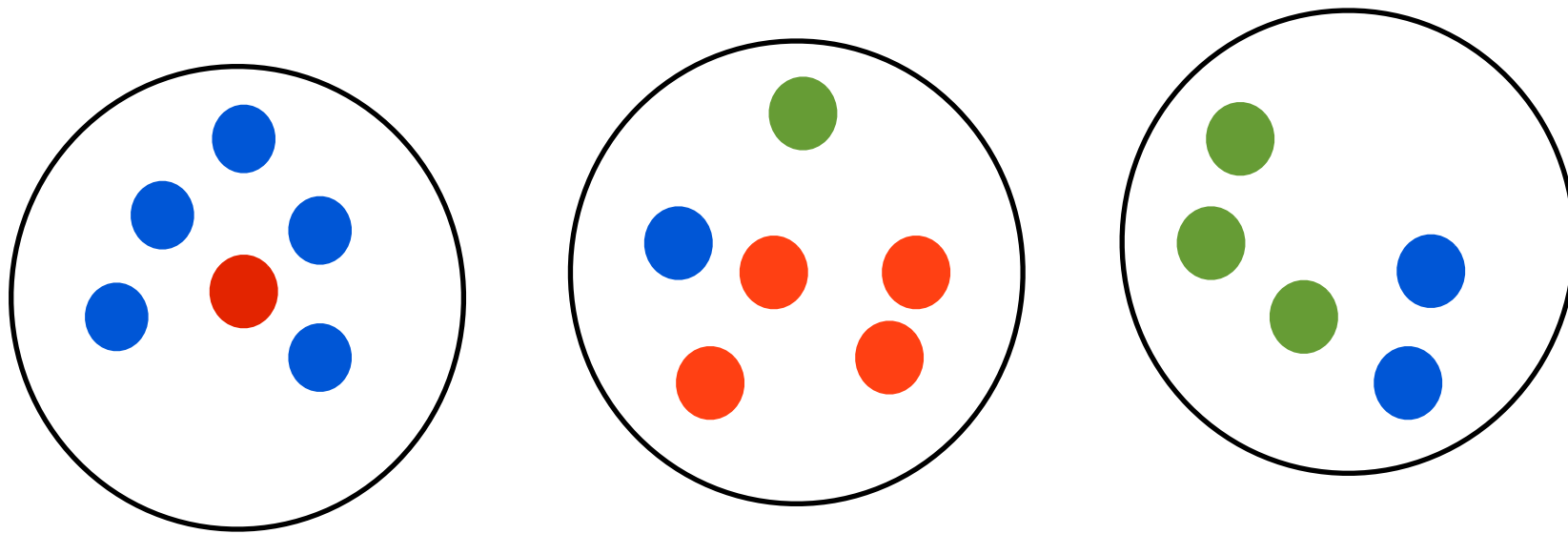
Evaluating Clustering — Rand Index (RI)

- Build a contingency table considering pairs of items in each cluster
 - Positive = same cluster
 - Negative = different clusters
 - True = same class
 - False = different classes
- TP = No. of item pairs that are in the same cluster and belong to the same class
- FP = No. of item pairs that are in the same cluster but belong to different classes
- TN = No. of item pairs that are in different clusters and belong to different classes
- FN = No. of item pairs that are in different clusters but belong to the same class

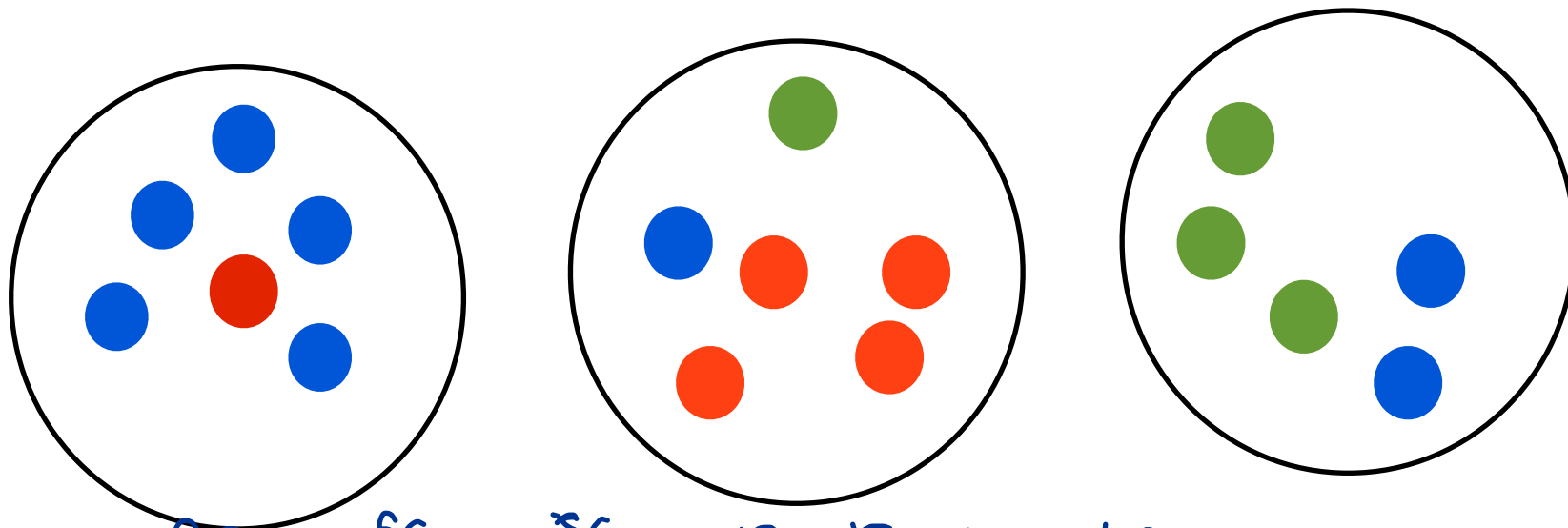
contingency table	same cluster	different clusters
same class	TP	FN
different classes	FP	TN

$$RI = \frac{TP + TN}{TP + FP + TN + FN}$$

(accuracy of
the clustering)



Quiz: Compute RI for this clustering.



$$TP + FP = {}^6C_2 + {}^6C_2 + {}^3C_2 = 15 + 15 + 10 = 40.$$

$$\downarrow$$

$$\left[{}^nC_r = \frac{n!}{r!(n-r)!} \right]$$

$${}^6C_2 = \frac{6!}{2!4!} = \frac{6 \times 5}{2} = 15 \quad {}^3C_2 = \frac{3!}{2!1!} = \frac{3 \times 2}{2} = 3.$$

$$TP = {}^5C_2 + {}^4C_2 + {}^3C_2 + {}^2C_2 = 10 + 6 + 3 + 1 = 20$$

$${}^4C_2 = \frac{4!}{2!2!} = \frac{4 \times 3}{2} = 6$$

$$\therefore FP = 40 - 20 = 20.$$

$$FN = (5 \times 1) + (1 \times 4) + (5 \times 2) + (1 \times 2) + (1 \times 3)$$

$$= 5 + 4 + 10 + 2 + 3 = 24$$

$$TN \neq FN = (5+1)(1+1+4) + (5+1)(3+2) + (1+1+4)(3+2)$$

$$= 6 \times 6 + 6 \times 5 + 6 \times 5 = 36 + 30 + 30 = 96.$$

$$\therefore TN = 96 - 24 = 72$$

	same cluster	different clusters
same class	20	24
different classes	20	72

$$RI = (20+72) / (20+24+20+72)$$

$$= 0.676$$

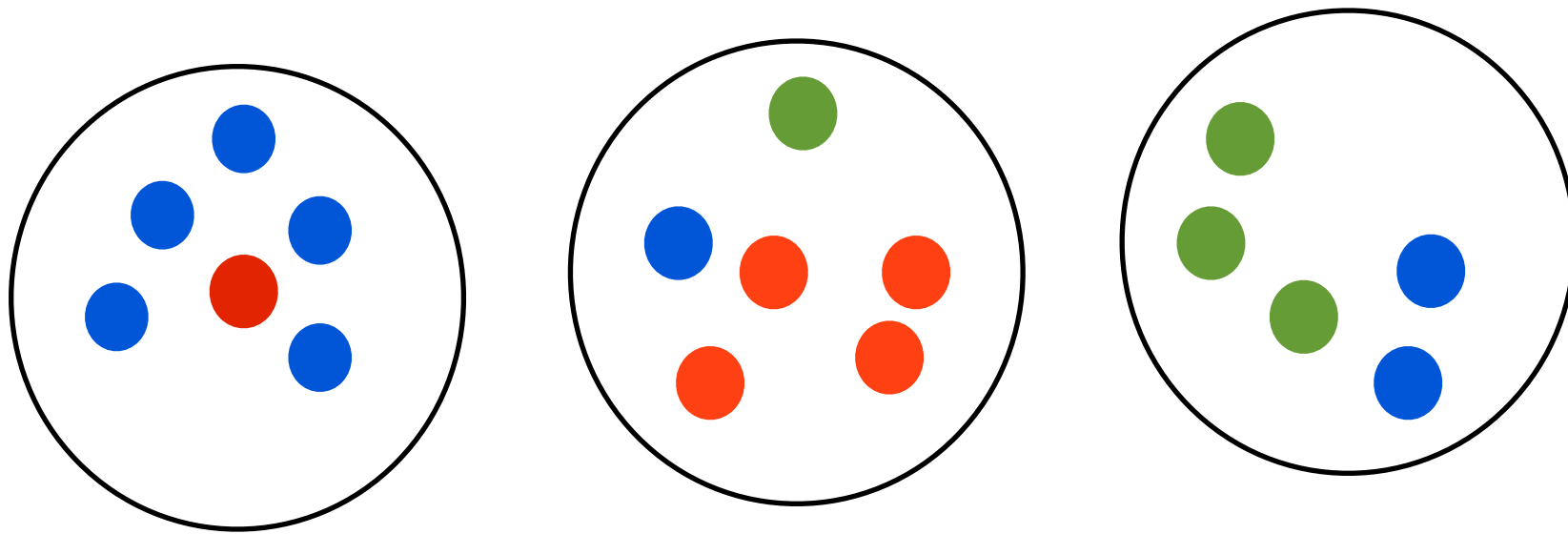
Evaluating Clustering — P/R/F

- We can use Precision (P), Recall (R), and F-measure (F) at to evaluate the accuracy of a clustering.
- For this purpose we must first create the contingency table as we did for RI and then compute P, R, F as follows

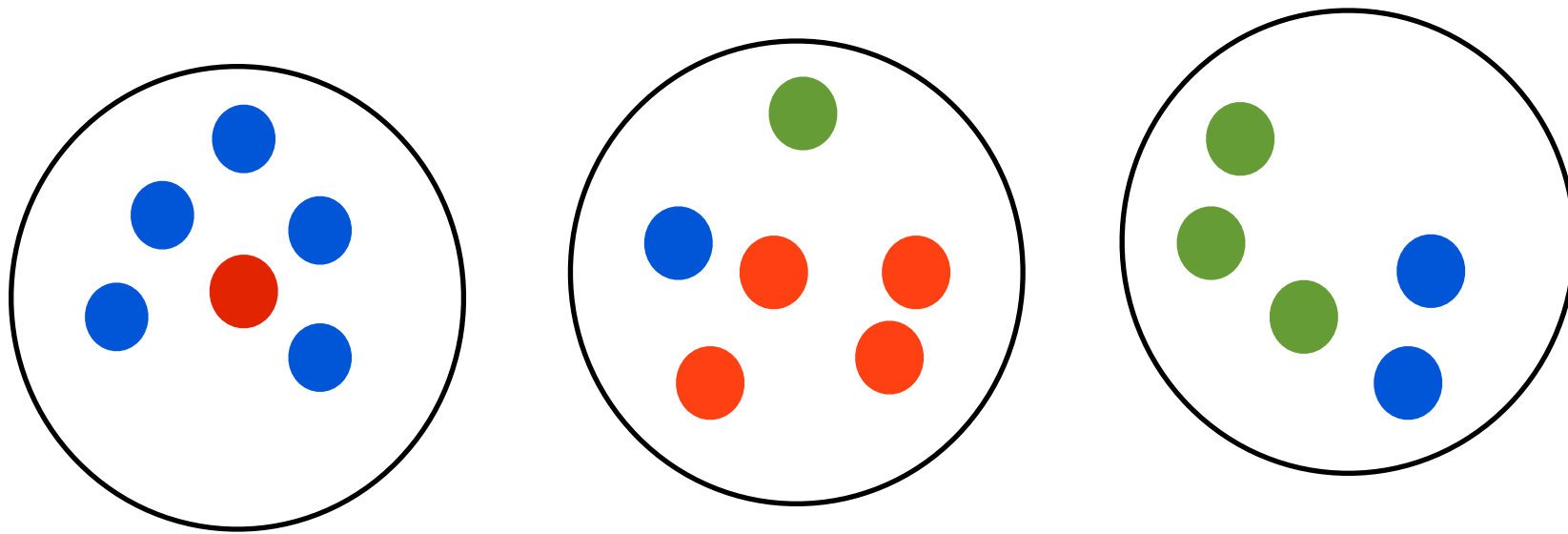
$$P = TP / (TP + FP)$$

$$R = TP / (TP + FN)$$

$$F = 2PR / (P + R)$$



Quiz: Compute P/R/F for this clustering.



	same cluster	different clusters
same class	TP=20	FN=24
different classes	FP=20	TN=72

$$P = TP / (TP + FP) = 20 / (20+20) = 0.5$$

$$R = TP / (TP + FN) = 20 / (20 + 24) = 0.45$$

$$F = 2PR / (P + R) = 0.47$$

B-CUBED Measure

- Proposed in (Bagga B. Baldwin = B^3)
 - A. Bagga and B. Baldwin. Entity-based cross document coreference resolution using the vector space model, In Proc. of 36th COLING-ACL, pages 79--85, 1998.
- We would like to evaluate clustering without labelling any clusters.

$$\text{precision}(x) = \frac{\text{No. of items in } C(x) \text{ with } A(x)}{\text{No. of items in } C(x)}$$

$$\text{recall}(x) = \frac{\text{No. of items in } C(x) \text{ with } A(x)}{\text{Total no. of items with } A(x)}$$

$C(x)$: The ID of the cluster that x belongs to

$A(x)$: label of x

B-CUBED Measure

- Compute the average over all the items (instances) that appear in all clusters (N)

$$\text{Precision} = \frac{1}{N} \sum_{p \in DataSet} \text{Precision}(p)$$

$$\text{Recall} = \frac{1}{N} \sum_{p \in DataSet} \text{Recall}(p)$$

$$F\text{-Score} = \frac{1}{N} \sum_{p \in DataSet} F(p)$$

Hierarchical Clustering

- Sometimes we might want to organise the data into a hierarchy of subsuming concepts for visualisation (abstraction) purposes
- Two methods exists
 - Conglomerative clustering
 - Start from one big cluster with all data instances and repeatedly partition it
 - Top-down approach
 - Agglomerative clustering
 - Start singletons (clusters with exactly one instance) and iteratively merge the most *similar* two clusters
 - Bottom-up approach
 - computationally more efficient ($O(\log n)$ merges required)

Merging two clusters

- Single linkage
 - Distance between two clusters A and B is the smallest distance between any instance $a \in A$ and $b \in B$

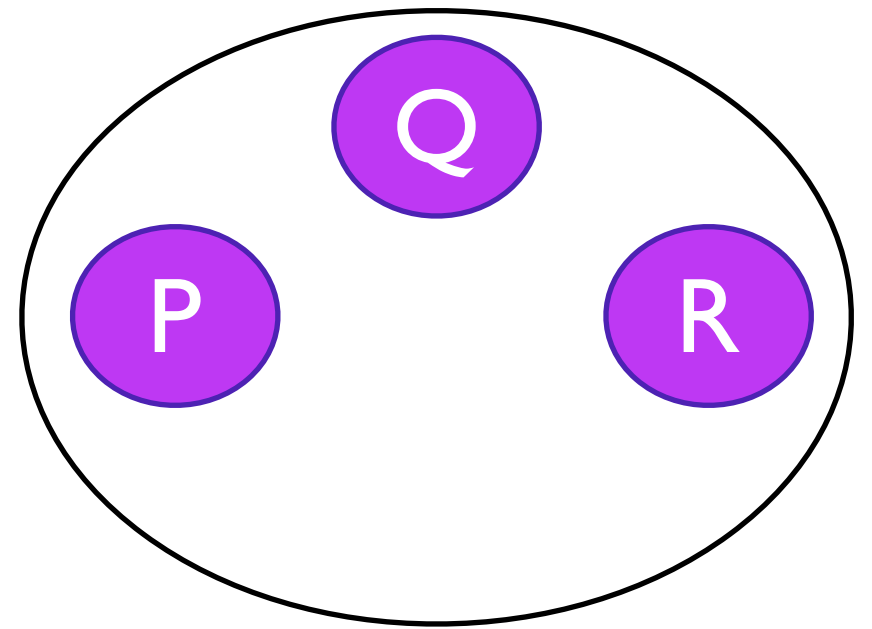
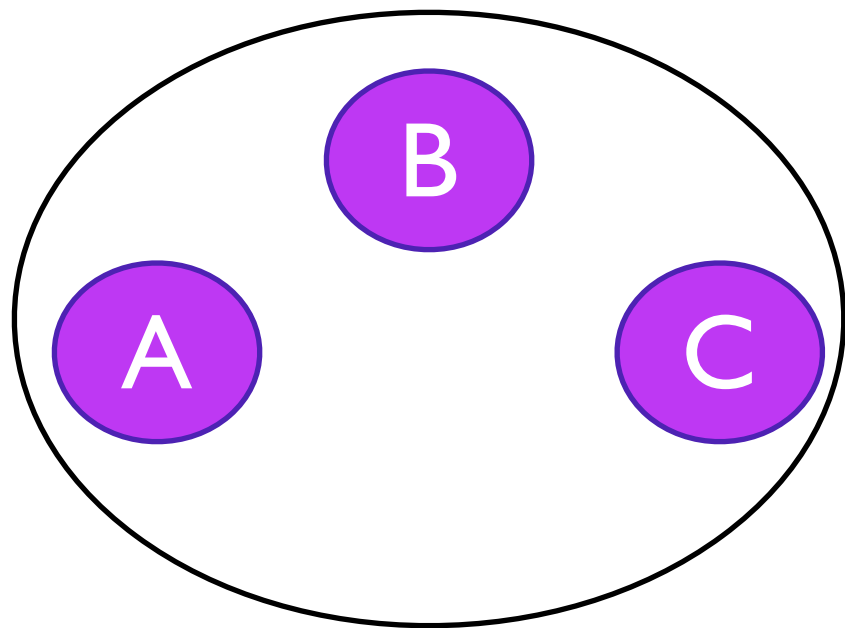
$$D(\mathcal{A}, \mathcal{B}) = \min_{a \in \mathcal{A}, b \in \mathcal{B}} dist(a, b)$$

- Complete linkage
 - Distance between two clusters A and B is the largest distance between any instance $a \in A$ and $b \in B$

$$D(\mathcal{A}, \mathcal{B}) = \max_{a \in \mathcal{A}, b \in \mathcal{B}} dist(a, b)$$

- Average linkage (Group-Average)
 - Average of all the pairs selected from each cluster

$$D(\mathcal{A}, \mathcal{B}) = \frac{1}{|\mathcal{A}||\mathcal{B}|} \sum_{a \in \mathcal{A}, b \in \mathcal{B}} dist(a, b)$$



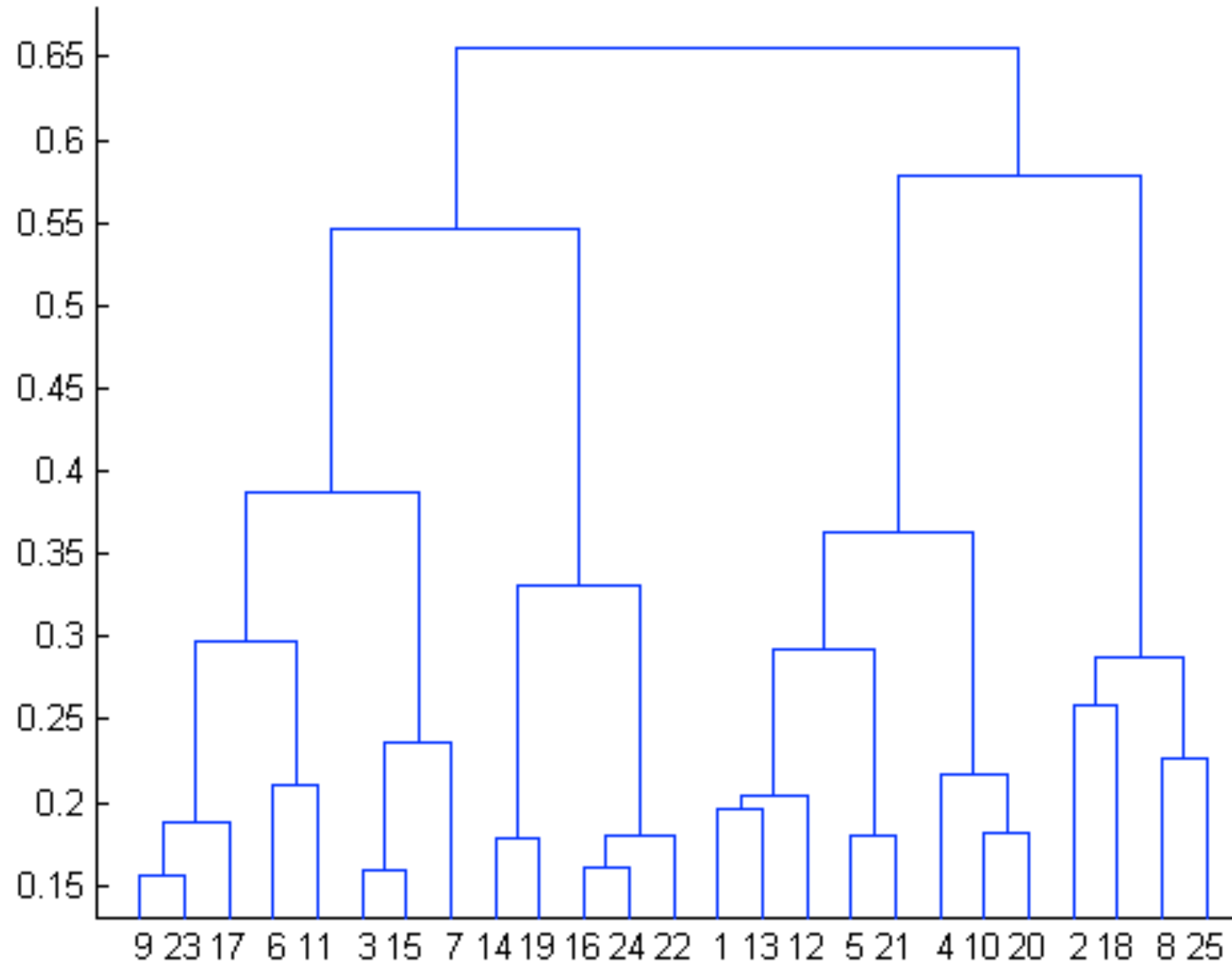
Quiz: Let us assume that in the 2D space there are two clusters $\{A, B, C\}$ and $\{P, Q, R\}$. Which of the distances correspond to the single link and complete link distances between the shown clusters?

Group-Average Agglomerative Clustering

- INPUT:
 - A set of N data instances $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, Number of clusters k
- Initialise
 - Create singletons $S_i = \{\mathbf{x}_i\}$ for $i = 1, \dots, N$
- Repeat until only we are left with one cluster
 - Merge the two clusters S_i and S_j with the minimum distance (cf. maximum similarity)

$$D(\mathcal{S}_i, \mathcal{S}_j) = \frac{1}{|\mathcal{S}_i||\mathcal{S}_j|} \sum_{a \in \mathcal{S}_i, b \in \mathcal{S}_j} dist(a, b)$$

Dendrogram



Clusters as Features

- We can use clustering to find *similar* features in instances without requiring any supervision (no label data is required for clustering)
 - Distributional similarity of features over instances
- Once we have clustered the features, we can use the cluster IDs as features
- Benefits
 - Reduces the dimensionality of the feature space
 - *dogs* and *cats* are mapped to *pets*
 - Reduces feature sparseness
 - If at least one of the features in a cluster appears in an instance, then we assume that the entire cluster appeared as a feature for that instance

Clustering the word-document Matrix

	d_1	d_2	d_3	d_4	d_5	d_6
dog	2	3	0	0	1	5
cat	1	1	0	0	3	2
apple	0	0	1	2	3	0
banana	0	0	2	5	0	0

Clustering the 2D matrix

- Each row vector can be seen as the feature vector for each word (row elements)
- We can measure similarity between row vectors and cluster the words
- Each column vector can be seen as the feature vector for each document (column elements)
- We can measure similarity between column vectors and cluster the documents

Co-clustering

- Cluster both rows and columns simultaneously!
 - You will get both row and column clusters
- Information Theoretic Co-Clustering (ITCC)
 - Inderjit Dhillon and Subramanyam Mallela and Dharmendra Modha, pp. 89--98, International Conference on Knowledge Discovery and Data Mining (KDD), 2003.

Clustering as Graph Partitioning

- Given a set of instances $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, we can represent these instances using a weighted undirected graph G , where the weight of the edge that connects two vertices in the graph corresponds to the similarity between the corresponding vertices.
- Then, the clustering problem becomes a graph partitioning problem where we must delete k edges from this graph to create k number of clusters
- Spectral clustering algorithms (discussed later at the lecture for Graph Mining)