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COMP3055 Machine Learning

Topic 9 – Data Clustering

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Supervised VS Unsupervised Learning

- Supervised learning
  - learning a function that maps an input to an output based on example input-output pairs.
  - training data is labeled.
- Unsupervised learning
  - learns from test data that has not been labeled.
  - learn relationships between elements in a data set and classify the raw data without "help."
  - Typical application includes data clustering.

Motivating Problems

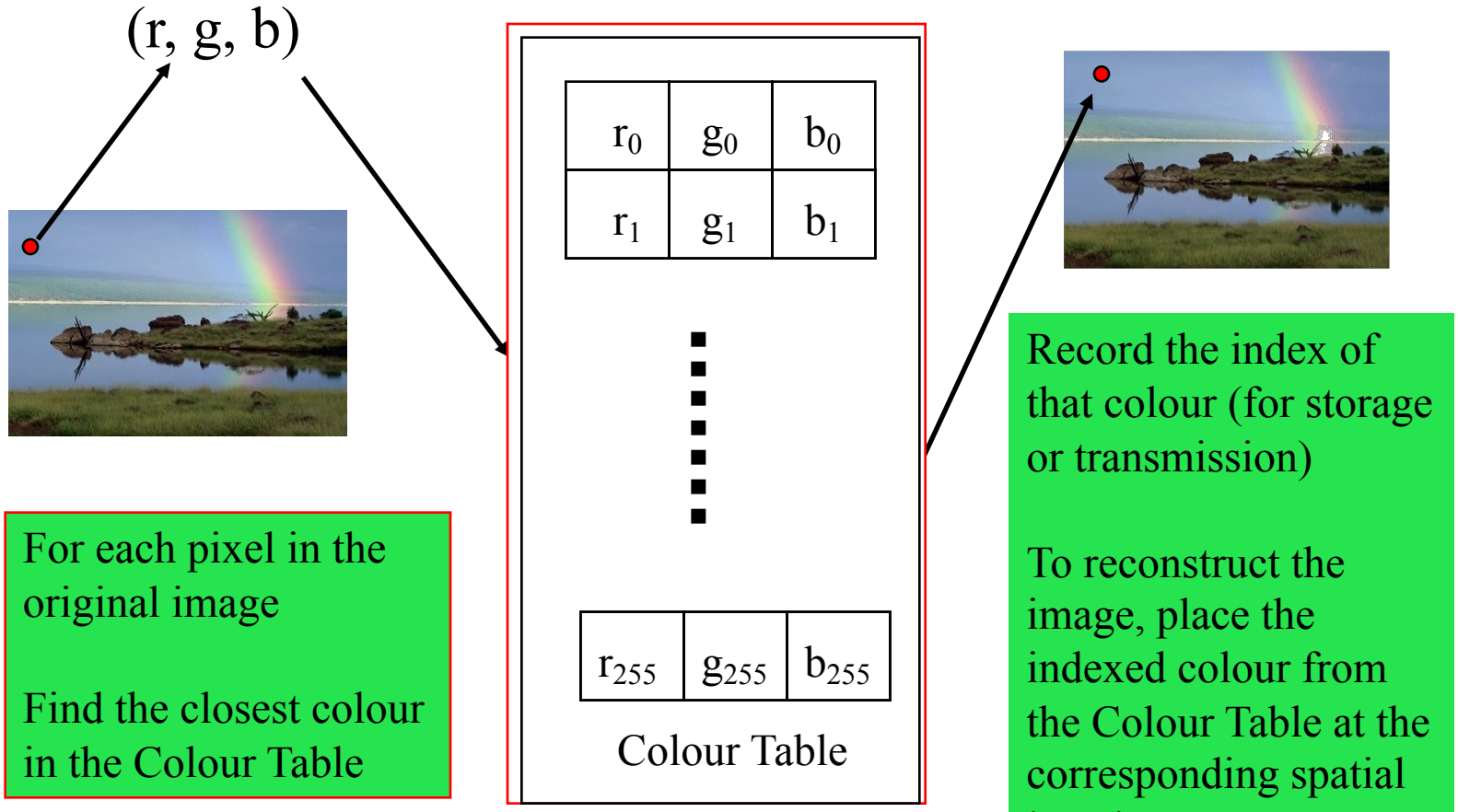
- A true colour image – 24bits/pixel, R – 8 bits, G – 8 bits, B – 8 bits

1677216 possible colours

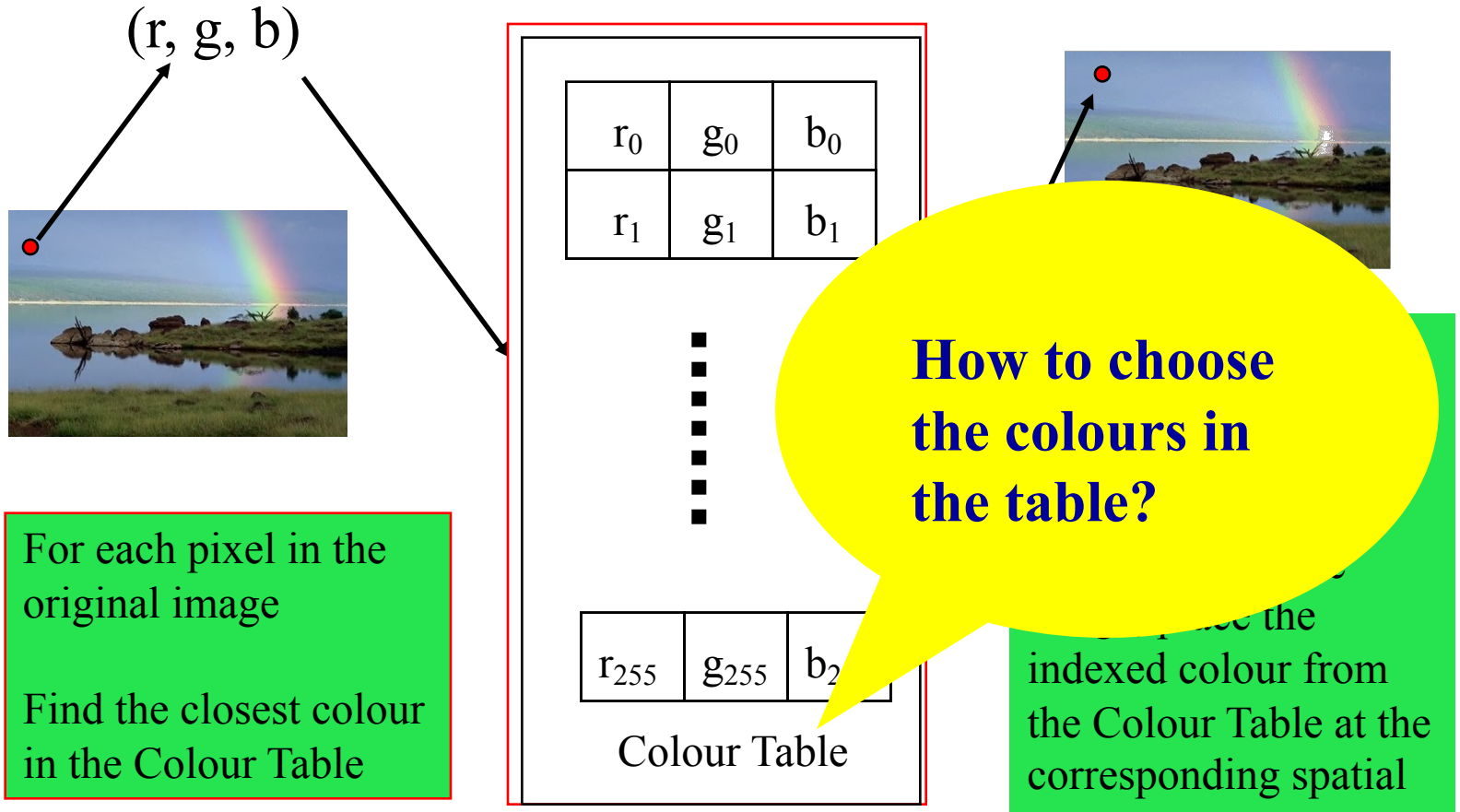
- A gif image - 8bits/pixel

256 possible colours

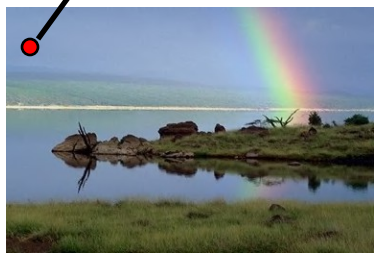
Motivating Problems



Motivating Problems



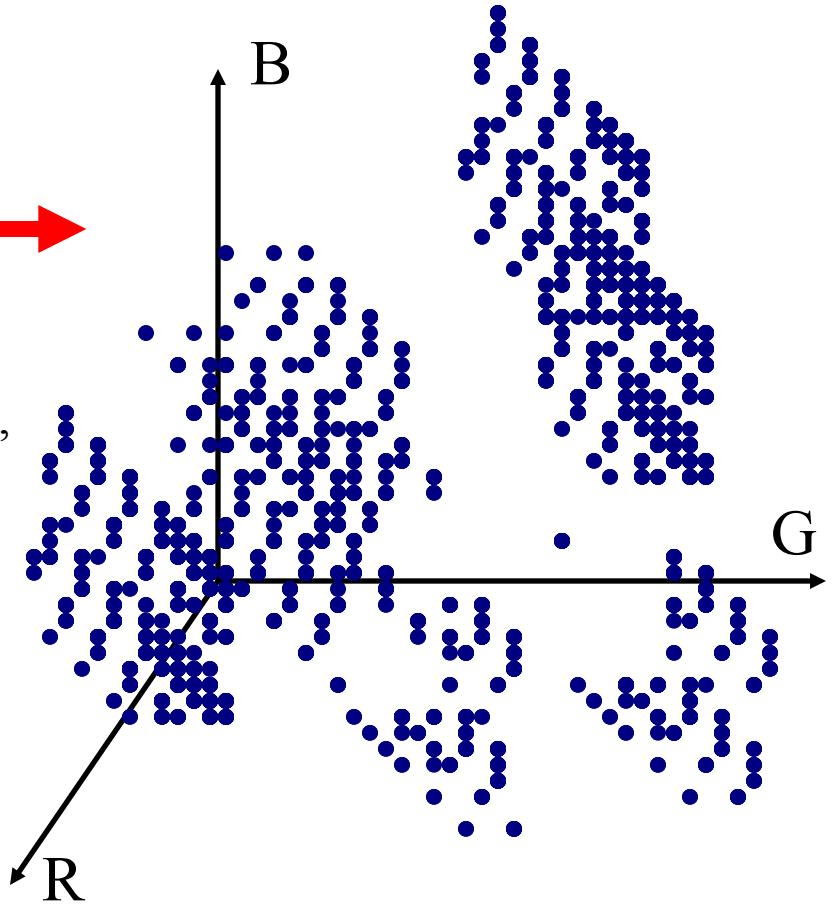
Motivating Problems



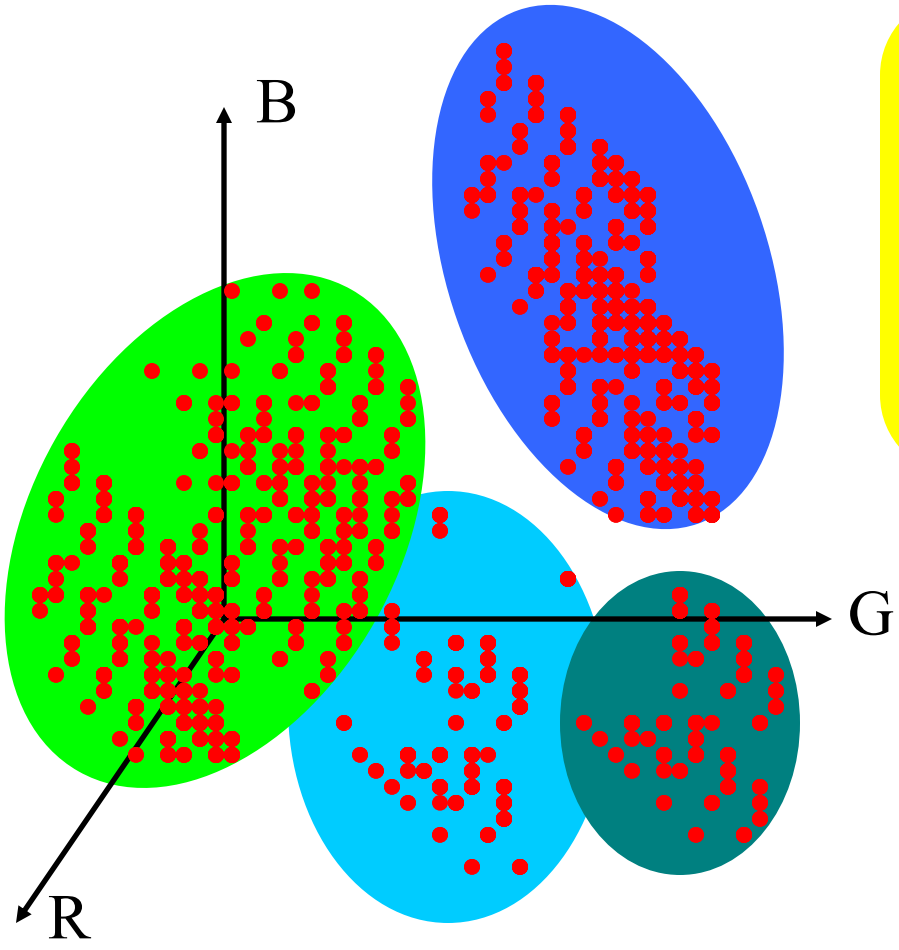
A pixel corresponding to
A point in the 3 dimensional
R, G, B space

Motivating Problems

Map all pixels into the R, G, B space, "clouds" of pixels are formed

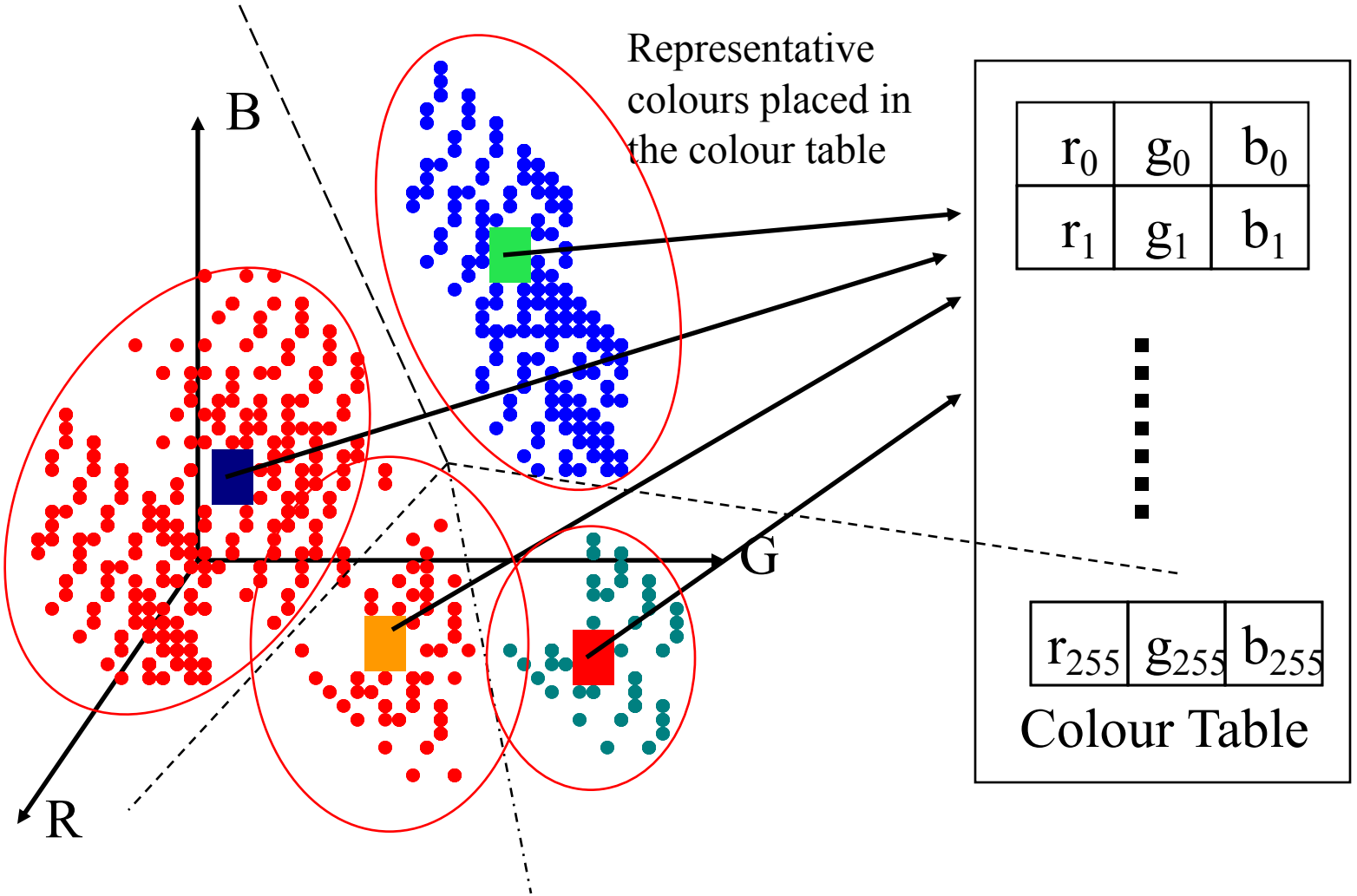


Motivating Problems



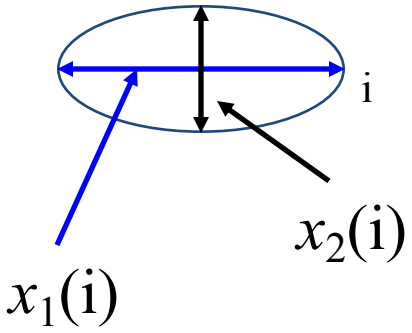
Group pixels that are close to each other, and replace them by one single colour

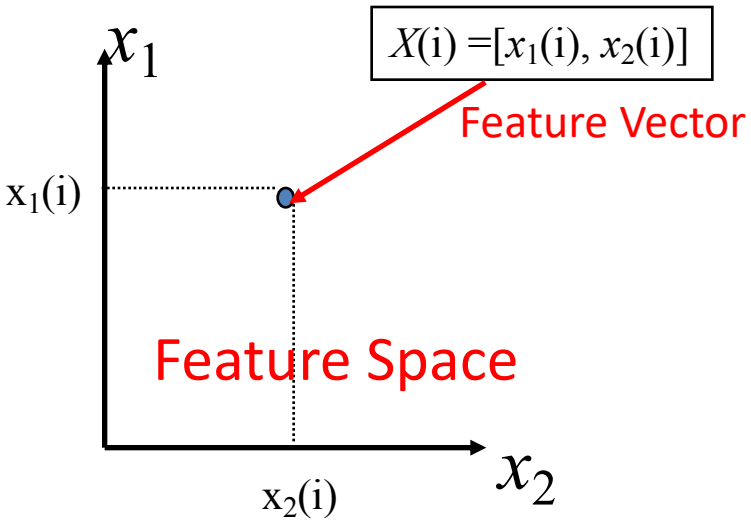
Motivating Problems

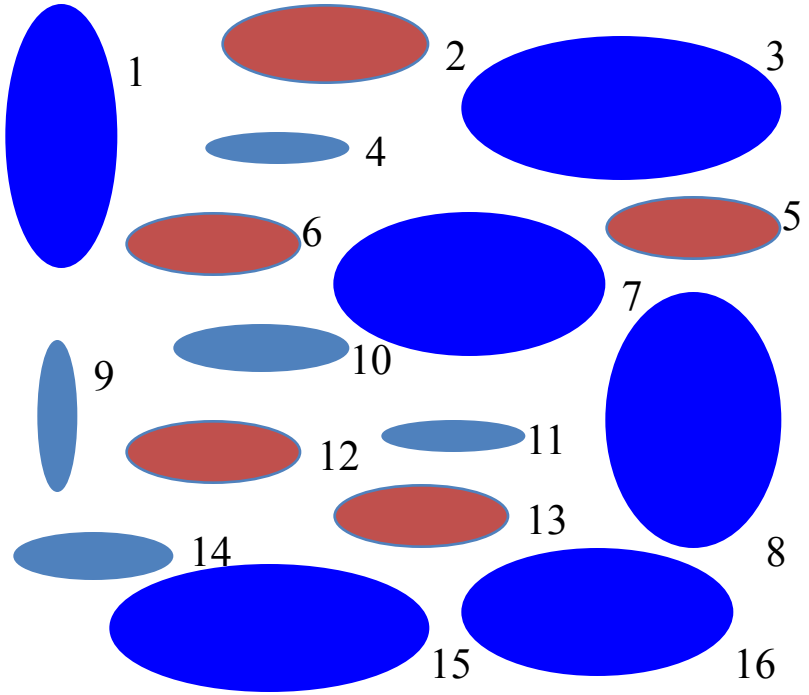


Motivating Example

- Classify objects (Oranges, Potatoes) into large, middle, small sizes



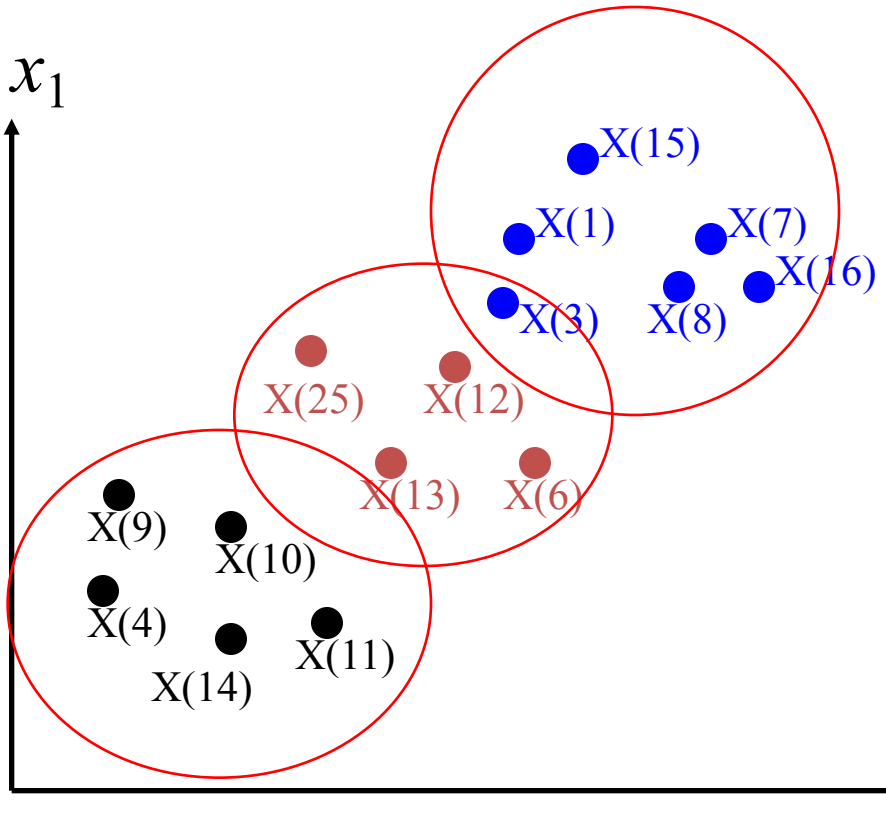


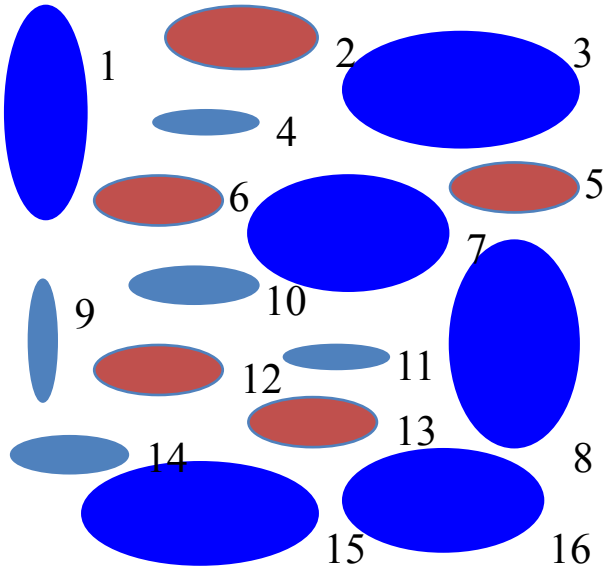


Elliptical blobs (objects)

Motivating Example

- From Objects to Feature Vectors to Points in the Feature Space





Elliptical blobs (objects)

Motivation of Clustering

- Patterns within a valid cluster are *more similar to each other* than they are to a pattern belonging to a different cluster.

- In clustering, the problem is to group a given collection of *unlabeled patterns* into meaningful clusters. Clustering is data *driven method*, the clusters are obtained solely from the data.

- Clustering could be used in the field of pattern-analysis, grouping, decision-making, and machine-learning situations, including data mining, document retrieval, image segmentation

K-Means

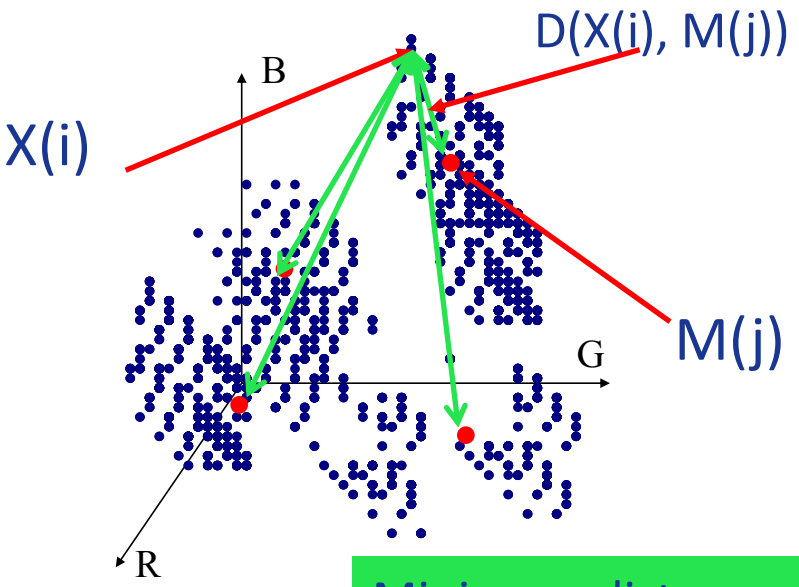
- An algorithm for partitioning (or clustering) N data points into K disjoint subsets S_j containing N_j data points
  - Define, $X(i) = [x_1(i), x_2(i), \ldots, x_n(i)]$, $i = 1, 2, \ldots N$, as N data points
  - We want to cluster these N points into K subsets, or K clusters, where K is pre-set
  - For each cluster, we define $M(j) = [m_1(j), m_2(j), \ldots, m_n(j)]$, $j=1, 2, \ldots K$, as its prototype or cluster centroids
  - Define the distance between data point X(i) and cluster prototype M(j) as

$$D\big(X(i),M(j)\big) = \big\|X(i)-M(j)\big\|^2 = \sum_{l=1}^{n}\big(x_l(i)-m_l(j)\big)^2$$

K-Means

- A data point X(i) is assigned to the jth cluster, C(j), X(i) $\in$ C(j), if following condition holds

$$D\big(X(i),M(j)\big)\leq D\big(X(i),M(l)\big) \quad \text{for all } l = 1, 2, ..., k$$



Minimum distance classifier

K-Means Algorithm

Step 1

- ✪ Arbitrarily choose from the given sample set k initial cluster centres,

$M^{(0)}(j) = [m^{(0)}_1(j), m^{(0)}_2(j), ,..., m^{(0)}_n(j)]$ $j = 1, 2, ..., K$,

e.g., the first K samples of the sample set
or can also be generated randomly

Set $t = 0$ (t is the iteration index)

K-Means Algorithm

Step 2

- Assign each of the samples X(i) = [x_1(i), x_2(i), …, x_n(i)], i = 1, 2, ….N, to one of the clusters according to the distance between the sample and the centre of the cluster:

$$X(i) \in C^{(t)}(j)$$
$$if \;\; D\left(X(i), M^{(t)}(j)\right) \leq D\left(X(i), M^{(t)}(l)\right)$$
$$\text{for all } l = 1, 2, \ldots, k$$

K-Means Algorithm

Step 3

Update the cluster centres to get

$M^{(t+1)}(j) = [m^{(t+1)}_1(j), m^{(t+1)}_2(j), ,..., m^{(t+1)}_n(j)]$; j = 1, 2, ..., K

according to

$$M^{(t+1)}(j) = \frac{1}{N_j^{(t)}} \sum_{X(i) \in C^{(t)}(j)} X(i)$$

$N^{(t)}_j$ is the number of samples in $C^{(t)}_j$

K-Means Algorithm

Step 4

– Calculate the error of approximation

$$E(t) = \frac{1}{2} \sum_{j=1}^{K} \sum_{X(i) \in C^{(t)}(j)} \left\| X(i) - M^{(t)}(j) \right\|^2$$

K-Means Algorithm

Step 5

– If the terminating criterion is met, then stop, otherwise

Set t = t+1

Go to Step 2.

K-Means Algorithm

Stopping criterions

- The K-means algorithm can be stopped based on following criterions

1. The errors do not change significantly in two consecutive epochs

   $|E(t)-E(t-1)|<\varepsilon$, where ε is some preset small value

2. No further change in the assignment of the data points to clusters in two consecutive epochs.

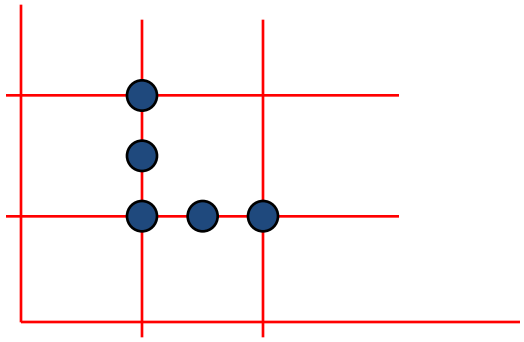
3. It can also stop after a fixed number of epochs regardless of the error

K-Means Algorithm

A worked example to see how it works exactly

Five 2-dimensional data points

(1, 1), (2, 1), (3, 1), (1, 2), (1, 3)



Cluster them into two clusters and find the cluster centres

K-Means Algorithm

- What is the algorithm doing exactly?
  - It tries to find the centre vectors M(j)'s that optimize the following cost function

$$E = \frac{1}{2}\sum_{j=1}^{K}\sum_{X(i)\in C(j)}\left\|X(i)-M(j)\right\|^2$$

K-Means Algorithm

- What is the algorithm doing exactly?

$$\frac{\partial E}{\partial m_l(j)} = \frac{\partial}{\partial m_l(j)}\left(\frac{1}{2}\sum_{j=1}^{K}\sum_{X(i)\in C(j)}\sum_{l=1}^{n}\left(x_l(i)-m_l(j)\right)^2\right)$$

$$= \frac{\partial}{\partial m_l(j)}\left(\frac{1}{2}\sum_{X(i)\in C(j)}\sum_{l=1}^{n}\left(x_l(i)-m_l(j)\right)^2\right)$$

$$= \sum_{X(i)\in C(j)}\left(x_l(i)-m_l(j)\right)\frac{\partial\left(x_l(i)-m_l(j)\right)}{\partial m_l(j)}$$

$$= -\sum_{X(i)\in C(j)}\left(x_l(i)-m_l(j)\right)$$

K-Means Algorithm

- What is the algorithm doing exactly?

$$\frac{\partial E}{\partial m_l(j)} = 0 \rightarrow -\sum_{X(i)\in C(j)} (x_l(i) - m_l(j)) = 0 \rightarrow \sum_{X(i)\in C(j)} x_l(i) = N_j m_l(j)$$

$$\rightarrow m_l(j) = \frac{1}{N_j} \sum_{X(i)\in C(j)} x_l(i) \rightarrow M(j) = \frac{1}{N_j} \sum_{X(i)\in C(j)} X(i)$$

K-means cluster centre updating rule (Step 3)

K-Means Algorithm

- Some remarks
  - Is a gradient descent algorithm, trying to minimize a cost function *E*
  - In general, the algorithm does not achieve a global minimum of E over the assignments.
  - Sensitive to initial choice of cluster centers. Different starting cluster centroids may lead to different solution
  - Is a popular method, many more advanced methods derived from this simple algorithm.