# $K$-means Clustering

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**Reading: [7.3, EA], [9.1, CMB]**

# Outline

- Introduction
- *K*-means Algorithm
- Example
- How *K*-means partitions?
- *K*-means Demo
- Relevant Issues
- Application: Cell Neulei Detection
- Summary

# Introduction

- Partitioning Clustering Approach
  - a typical clustering analysis approach via iteratively partitioning training data set to learn a partition of the given data space
  - learning a partition on a data set to produce several non-empty clusters (usually, the number of clusters given in advance)
  - in principle, optimal partition achieved via minimising the sum of squared distance to its "representative object" in each cluster

$$E = \sum_{k=1}^{K} \sum_{\mathbf{x} \in C_k} d^2(\mathbf{x}, \mathbf{m}_k)$$

e.g., Euclidean distance $d^2(\mathbf{x}, \mathbf{m}_k) = \sum_{n=1}^{N} (x_n - m_{kn})^2$

# Introduction

- Given a *K*, find a partition of *K clusters* to optimise the chosen partitioning criterion (cost function)
  - o global optimum: exhaustively search all partitions
- The *K-means* algorithm: a heuristic method
  - o K-means algorithm (MacQueen'67): each cluster is represented by the centre of the cluster and the algorithm converges to stable centriods of clusters.
  - o K-means algorithm is the simplest partitioning method for clustering analysis and widely used in data mining applications.

# K-means Algorithm

- Given the cluster number *K*, the *K-means* algorithm is carried out in three steps after initialisation:

Initialisation: set seed points (randomly)

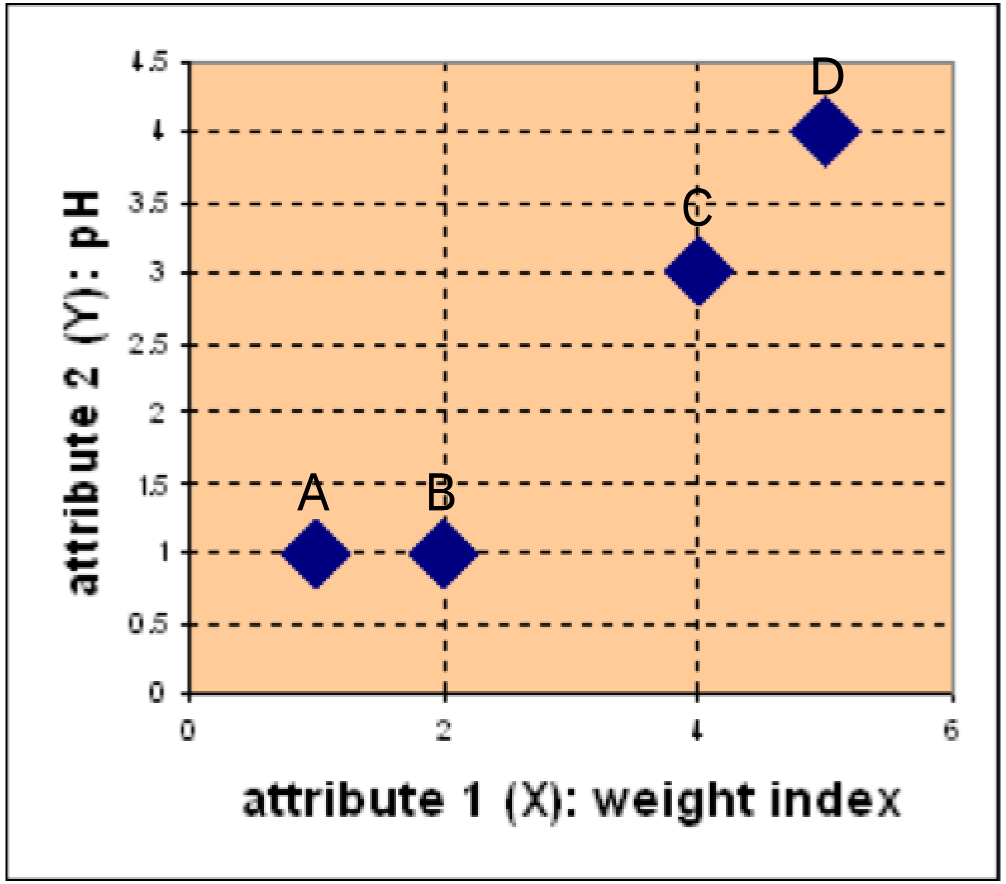
1) Assign each object to the cluster of the nearest seed point measured with a specific distance metric
2) Compute new seed points as the centroids of the clusters of the current partition (the centroid is the centre, i.e., *mean point*, of the cluster)
3) Go back to Step 1), stop when no more new assignment (i.e., membership in each cluster no longer changes)

# Example

- Problem

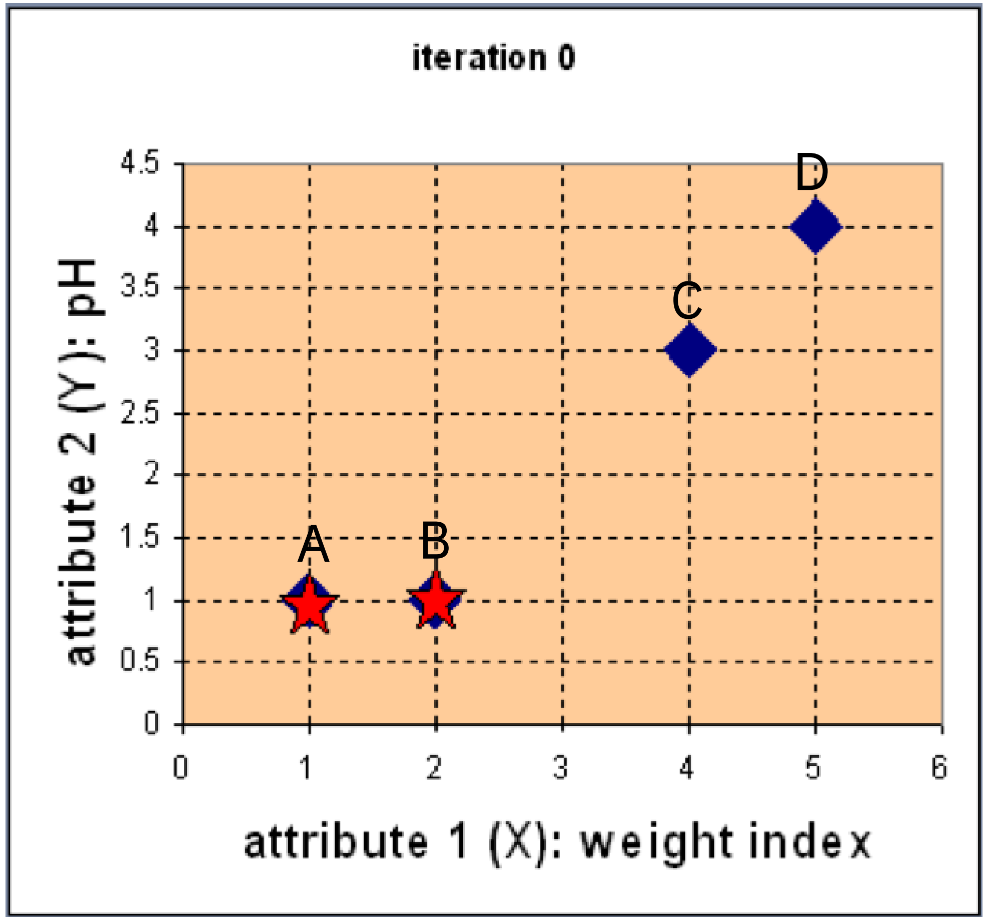
  Suppose we have 4 types of medicines and each has two attributes (pH and weight index). Our goal is to group these objects into *K=2* group of medicine.

| Medicine | Weight | pH-Index |
|---|---|---|
| A | 1 | 1 |
| B | 2 | 1 |
| C | 4 | 3 |
| D | 5 | 4 |



# Example

- Step 1: Use initial seed points for partitioning




$$\mathrm{c}_1 = \mathrm{A}, \mathrm{c}_2 = \mathrm{B}$$

$$\mathbf{D}^0 = \begin{array}{c} \begin{bmatrix} 0 & 1 & 3.61 & \boxed{5} \\ 1 & 0 & 2.83 & \boxed{4.24} \end{bmatrix} \\ \begin{matrix} A & B & C & D \end{matrix} \end{array} \qquad \begin{matrix} \mathbf{c}_1 = (1,1) & group-1 \\ \mathbf{c}_2 = (2,1) & group-2 \end{matrix}$$

Euclidean distance

$$\begin{array}{cc} \begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} & \begin{matrix} X \\ Y \end{matrix} \end{array}$$

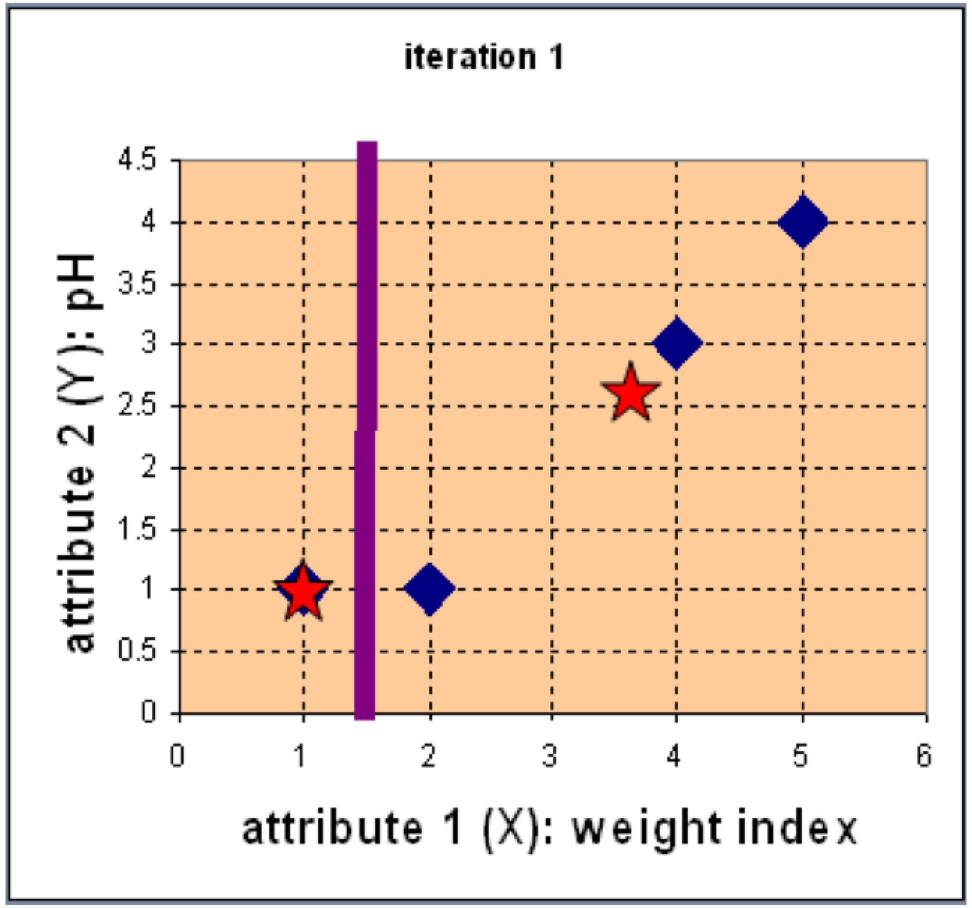
$$d(D,c_1) = \sqrt{(5-1)^2 + (4-1)^2} = 5$$

$$d(D,c_2) = \sqrt{(5-2)^2 + (4-1)^2} = 4.24$$

Assign each object to the cluster with the nearest seed point

# Example

- Step 2: Compute new centroids of the current partition




Knowing the members of each cluster, now we compute the new centroid of each group based on these new memberships.

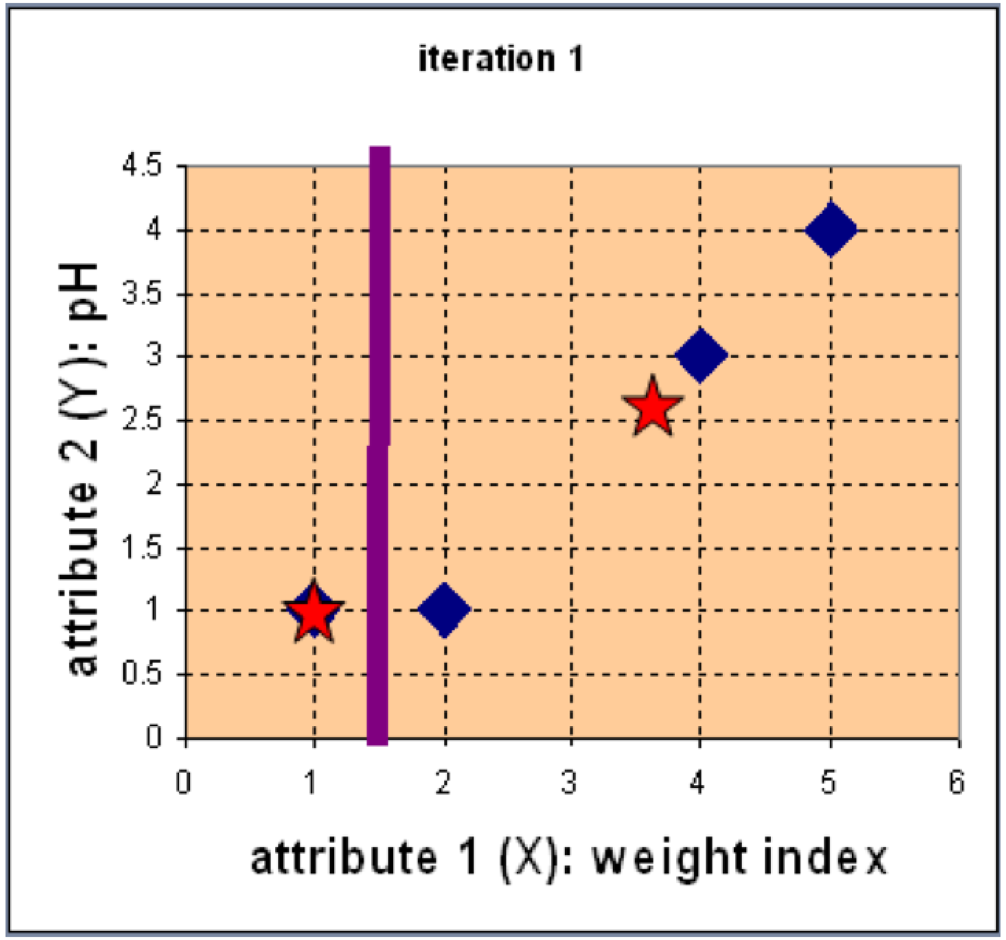
$$c_1 = (1,\ 1)$$

$$c_2 = \left(\frac{2+4+5}{3},\ \frac{1+3+4}{3}\right)$$

$$= \left(\frac{11}{3},\ \frac{8}{3}\right)$$

# Example

- Step 2: Renew membership based on new centroids




Compute the distance of all objects to the new centroids

$$\mathbf{D}^1 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 3.14 & 2.36 & 0.47 & 1.89 \end{bmatrix} \quad \begin{array}{ll} \mathbf{c}_1 = (1,1) & group-1 \\ \mathbf{c}_2 = (\frac{11}{3}, \frac{8}{3}) & group-2 \end{array}$$

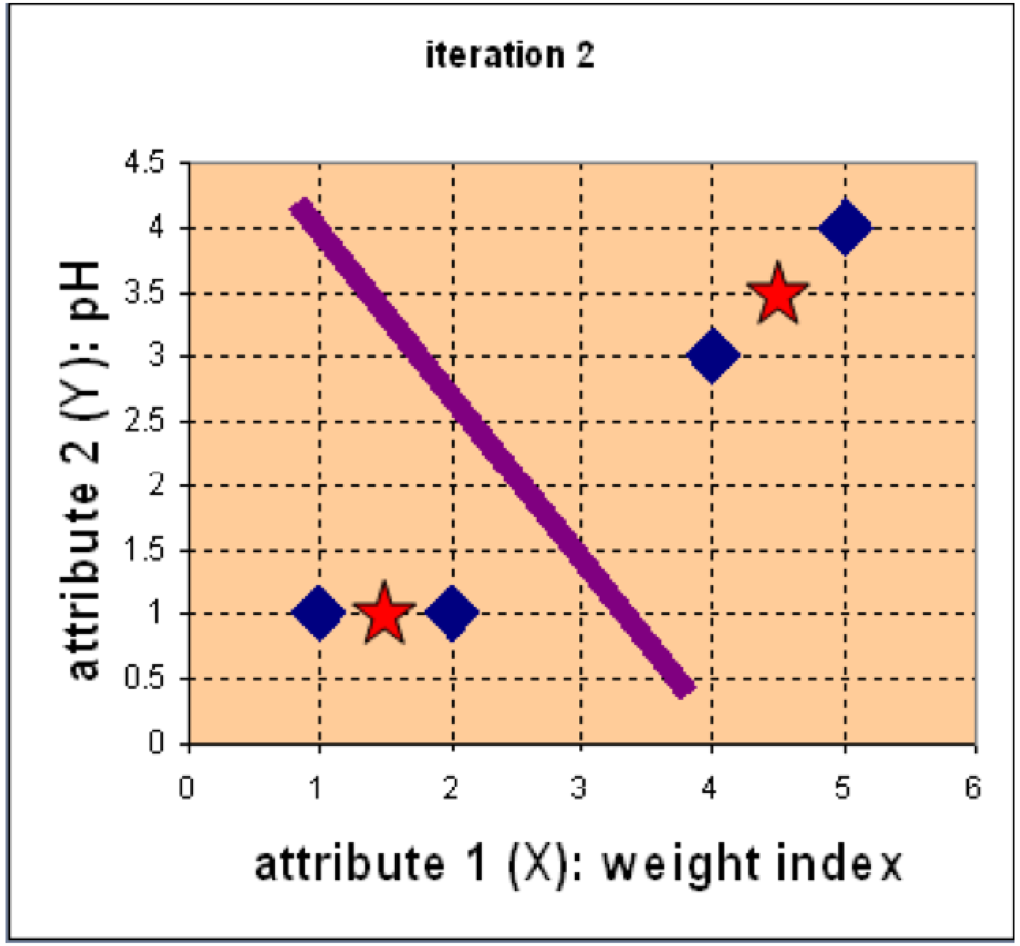
$$\begin{array}{cccc} A & B & C & D \end{array}$$

$$\begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} \begin{array}{l} X \\ Y \end{array}$$

Assign the membership to objects

# Example

- Step 3: Repeat the first two steps until its convergence



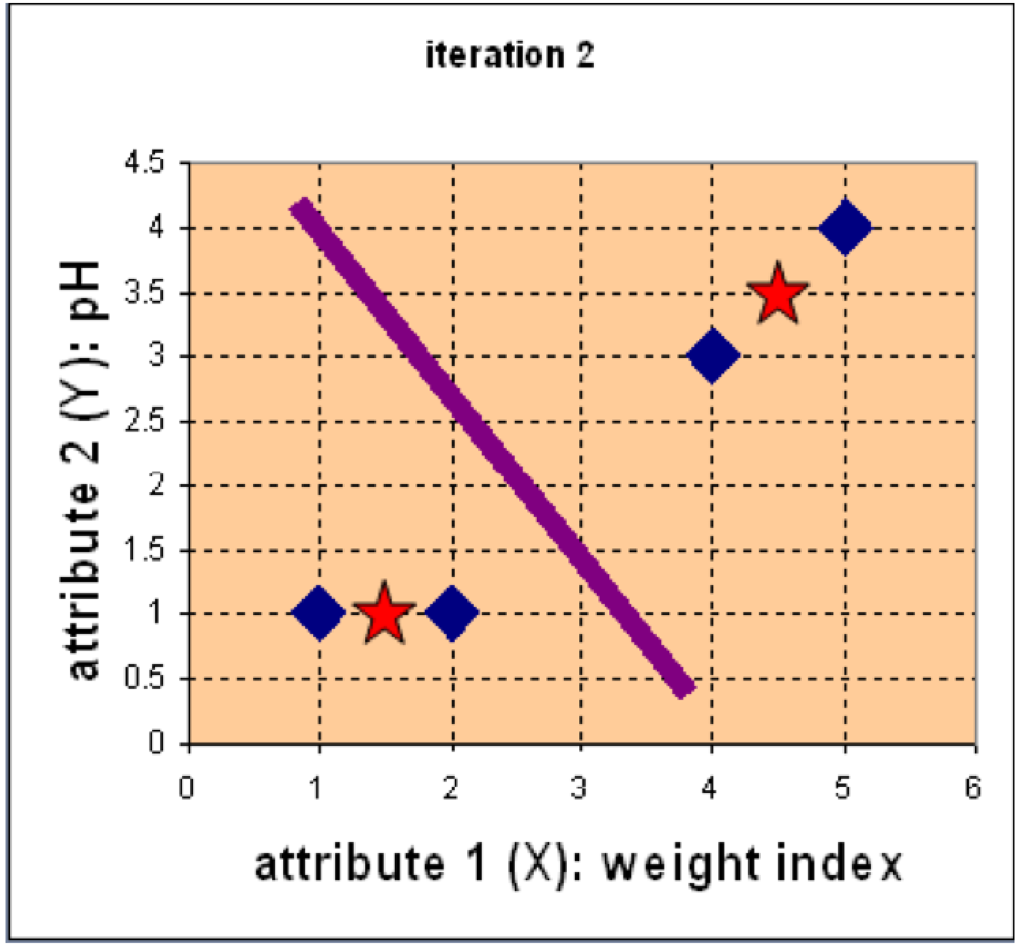

Knowing the members of each cluster, now we compute the new centroid of each group based on these new memberships.

$$c_1 = \left(\frac{1+2}{2}, \frac{1+1}{2}\right) = (1\frac{1}{2}, 1)$$

$$c_2 = \left(\frac{4+5}{2}, \frac{3+4}{2}\right) = (4\frac{1}{2}, 3\frac{1}{2})$$

# Example

- Step 3: Repeat the first two steps until its convergence




Compute the distance of all objects to the new centroids

$$\mathbf{D}^2 = \begin{bmatrix} 0.5 & 0.5 & 3.20 & 4.61 \\ 4.30 & 3.54 & 0.71 & 0.71 \end{bmatrix} \quad \begin{array}{ll} \mathbf{c}_1 = (1\tfrac{1}{2}, 1) & group-1 \\ \mathbf{c}_2 = (4\tfrac{1}{2}, 3\tfrac{1}{2}) & group-2 \end{array}$$

$$\begin{array}{cc} \begin{array}{cccc} A & B & C & D \end{array} & \\ \begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} & \begin{array}{c} X \\ Y \end{array} \end{array}$$

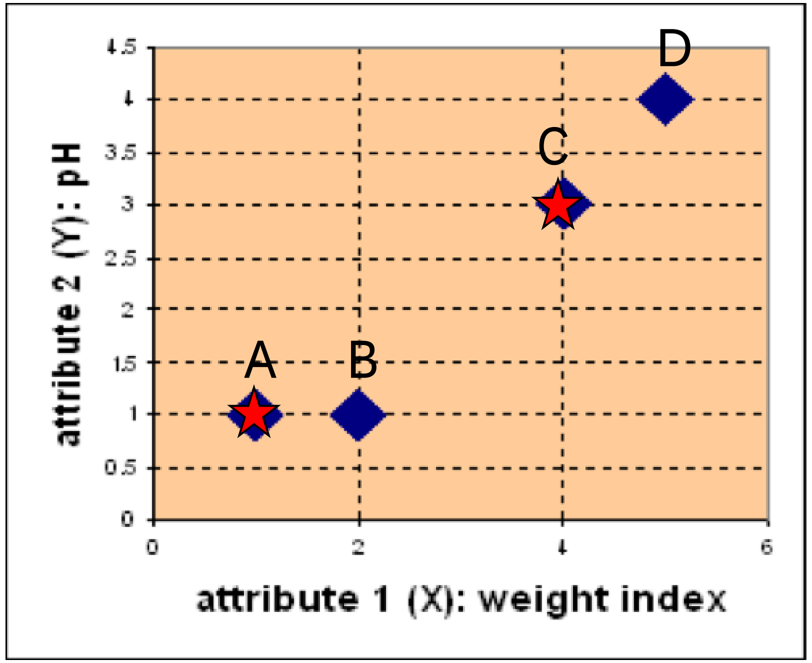
Stop due to no new assignment Membership in each cluster no longer change

# Exercise

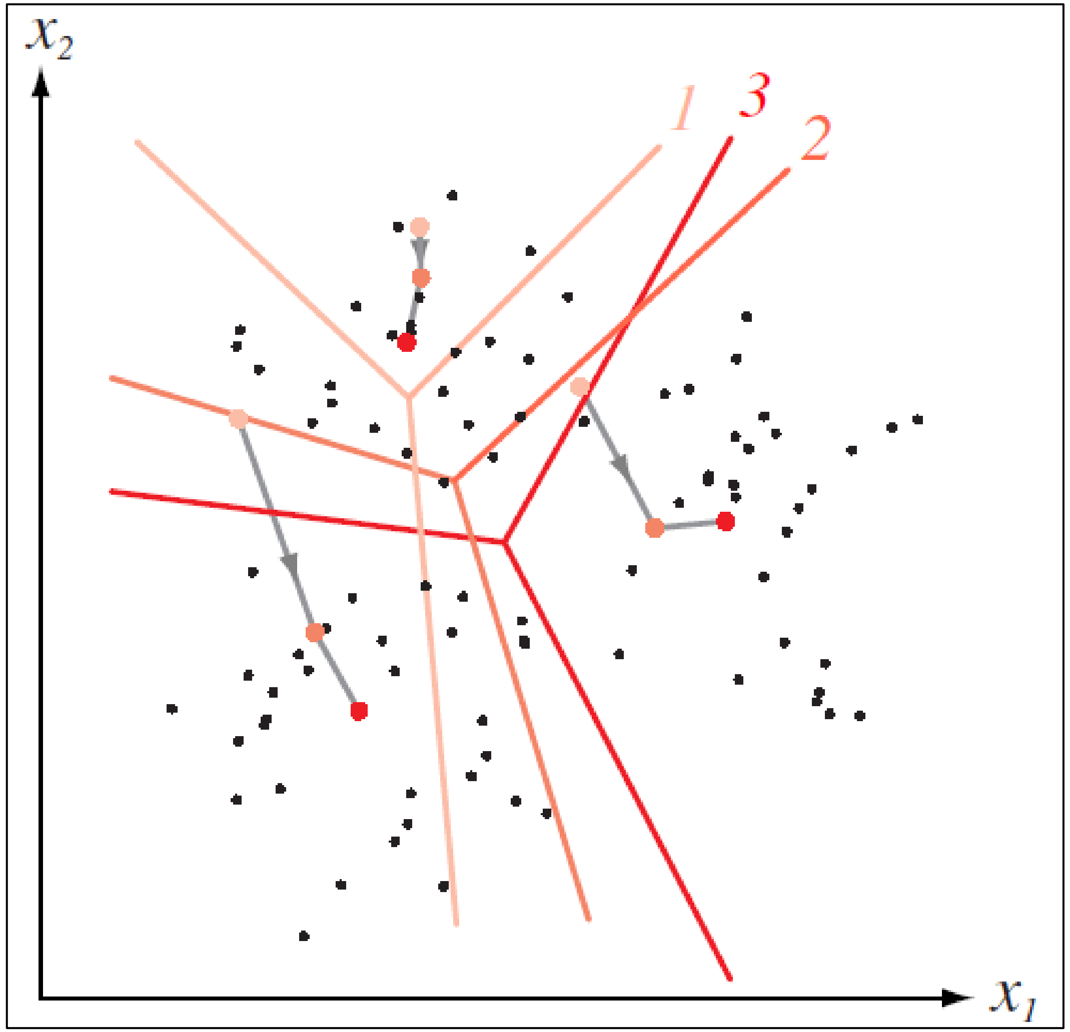
For the medicine data set, use K-means with the Manhattan distance metric for clustering analysis by setting $K$=2 and initialising seeds as $C_1$ = A and $C_2$ = C. Answer three questions as follows:

1. How many steps are required for convergence?
2. What are memberships of two clusters after convergence?
3. What are centroids of two clusters after convergence?

| Medicine | Weight | pH-Index |
|---|---|---|
| A | 1 | 1 |
| B | 2 | 1 |
| C | 4 | 3 |
| D | 5 | 4 |



# How K-means partitions?



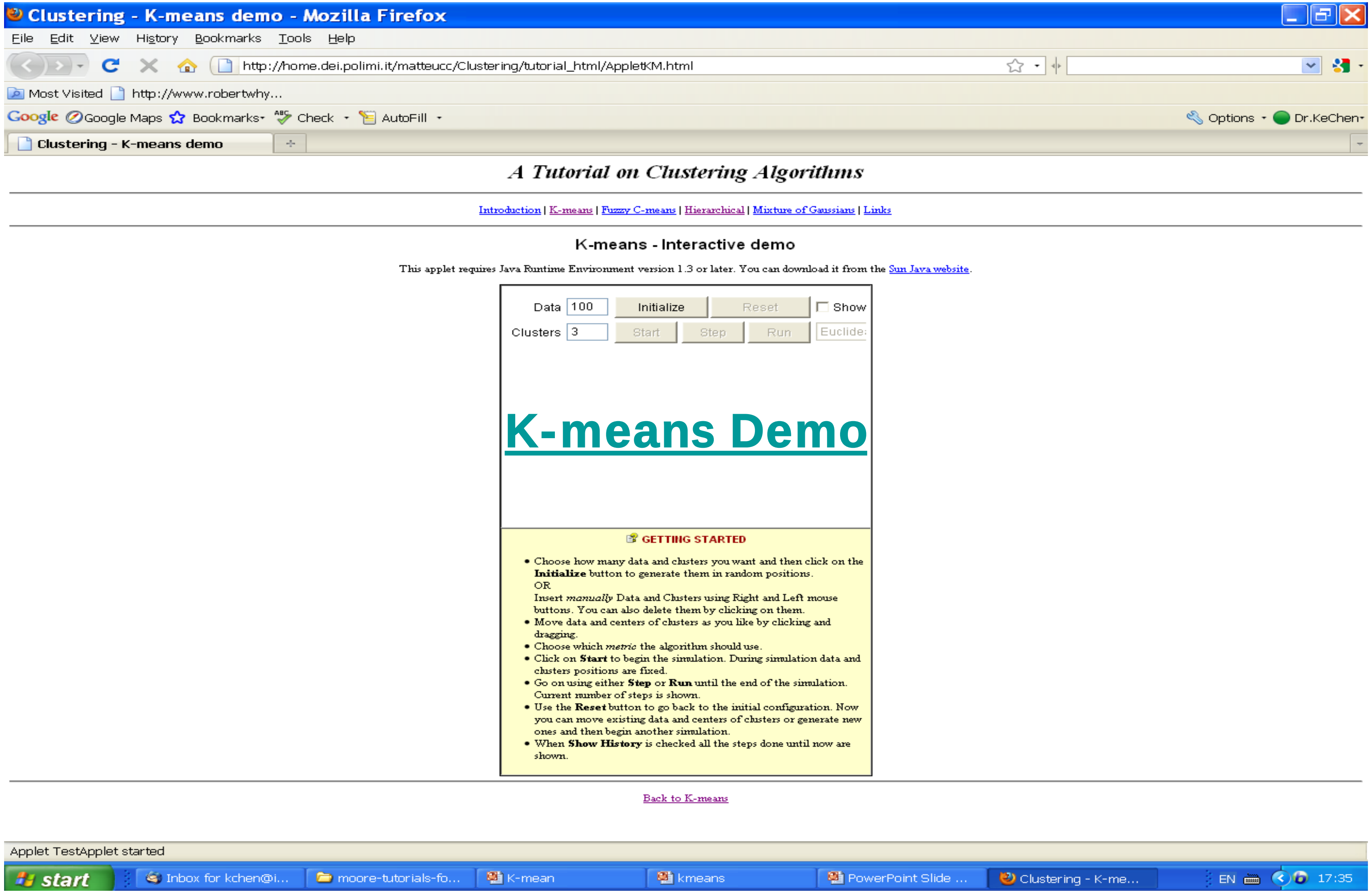

When $K$ centroids are set/fixed, they partition the whole data space into $K$ mutually exclusive subspaces to form a partition.

A partition amounts to a

[Voronoi Diagram]

Changing positions of centroids leads to a new partitioning.

# K-means Demo


Clustering - K-means demo - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://home.dei.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html
Most Visited http://www.robertwhy...
Google Google Maps Bookmarks Check AutoFill Options Dr.KeChen
Clustering - K-means demo
A Tutorial on Clustering Algorithms
Introduction | K-means | Fuzzy C-means | Hierarchical | Mixture of Gaussians | Links
K-means - Interactive demo
This applet requires Java Runtime Environment version 1.3 or later. You can download it from the Sun Java website.
Data 100 Initialize Reset Show
Clusters 3 Start Step Run Euclide
K-means Demo
GETTING STARTED
Choose how many data and clusters you want and then click on the Initialize button to generate them in random positions.
OR
Insert manually Data and Clusters using Right and Left mouse buttons. You can also delete them by clicking on them.
Move data and centers of clusters as you like by clicking and dragging.
Choose which metric the algorithm should use.
Click on Start to begin the simulation. During simulation data and clusters positions are fixed.
Go on using either Step or Run until the end of the simulation. Current number of steps is shown.
Use the Reset button to go back to the initial configuration. Now you can move existing data and centers of clusters or generate new ones and then begin another simulation.
When Show History is checked all the steps done until now are shown.
Back to K-means
Applet TestApplet started
start Inbox for kchen@i... moore-tutorials-fo... K-mean kmeans PowerPoint Slide ... Clustering - K-me... EN 17:35

# Relevant Issues

- Computational complexity
  - O($tKn$), where $n$ is number of objects, $K$ is number of clusters, and $t$ is number of iterations. Normally, $K$, $t << n$.
- Local optimum
  - sensitive to initial seed points
  - converge to a local optimum: maybe an unwanted solution
- Other problems
  - Need to specify *K,* the *number* of clusters, in advance
  - Unable to handle noisy data and outliers (*K-Medoids* algorithm)
  - Not suitable for discovering clusters with non-convex shapes
  - Applicable only when mean is defined, then what about categorical data? (*K-mode* algorithm)
  - how to evaluate the *K*-mean performance?

# Application

- Colour-Based Image Segmentation Using *K*-means

**Step 1**: Loading a colour image of tissue stained with hemotoxylin and eosin (H&E)

H&E image

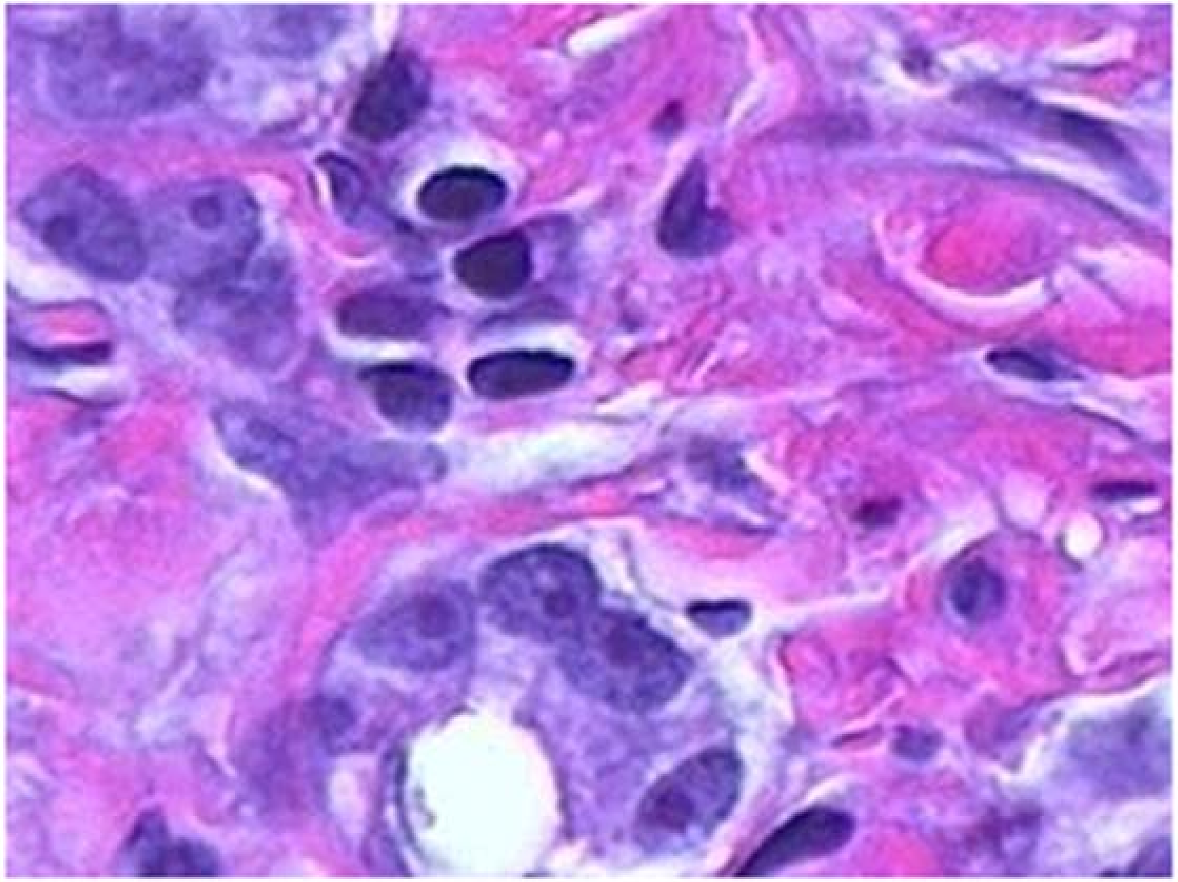


Image courtesy of Alan Partin, Johns Hopkins University

# Application

- [Colour-Based Image Segmentation Using *K*-means]

**Step 2**: Convert the image from RGB colour space to L*a*b* colour space

  - Unlike the RGB colour model, L*a*b* colour is designed to approximate human vision.
  - There is a complicated transformation between RGB and L*a*b*.

$$(L^*, a^*, b^*) = T(R, G, B).$$

$$(R, G, B) = T'(L^*, a^*, b^*).$$

# Application

- Colour-Based Image Segmentation Using *K*-means

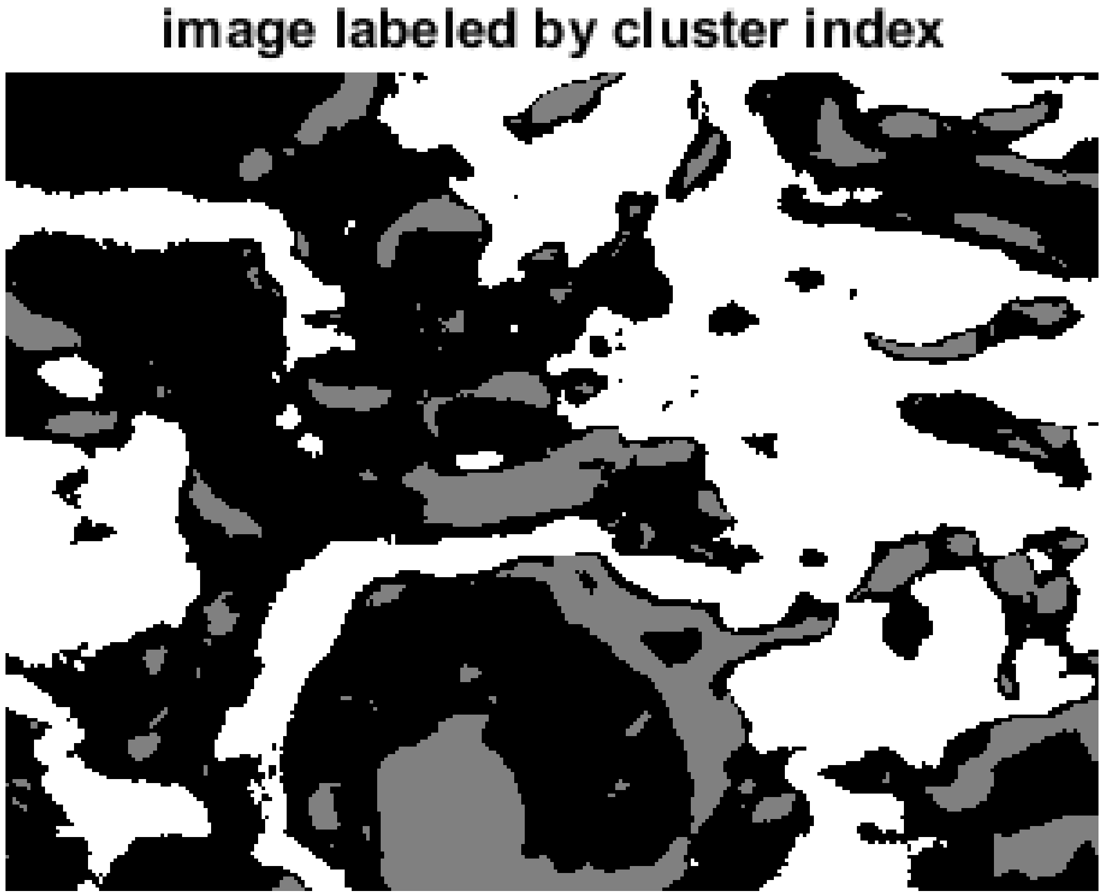
**Step 3**: Undertake clustering analysis in the (a*, b*) colour space with the *K*-means algorithm

- In the L*a*b* colour space, each pixel has a properties or feature vector: (L*, a*, b*).
- Like feature selection, L* feature is discarded. As a result, each pixel has a feature vector (a*, b*).
- Applying the *K*-means algorithm to the image in the a*b* feature space where $K = 3$ by applying the domain knowledge.

# Application

- Colour-Based Image Segmentation Using *K*-means

**Step 4**: Label every pixel in the image using the results from *K*-means clustering (indicated by three different grey levels)

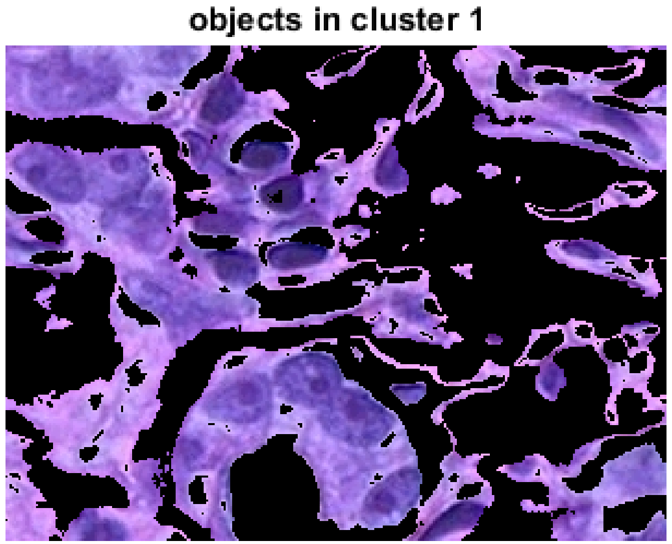


# Application

- [Colour-Based Image Segmentation Using *K*-means](#)

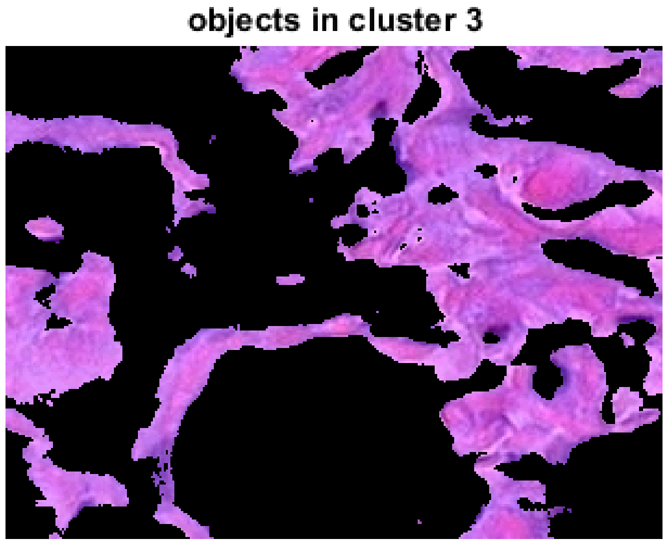
**Step 5**: Create Images that Segment the H&E Image by Colour

  - Apply the label and the colour information of each pixel to achieve separate colour images corresponding to three clusters.




“blue” pixels


“white” pixels




“pink” pixels

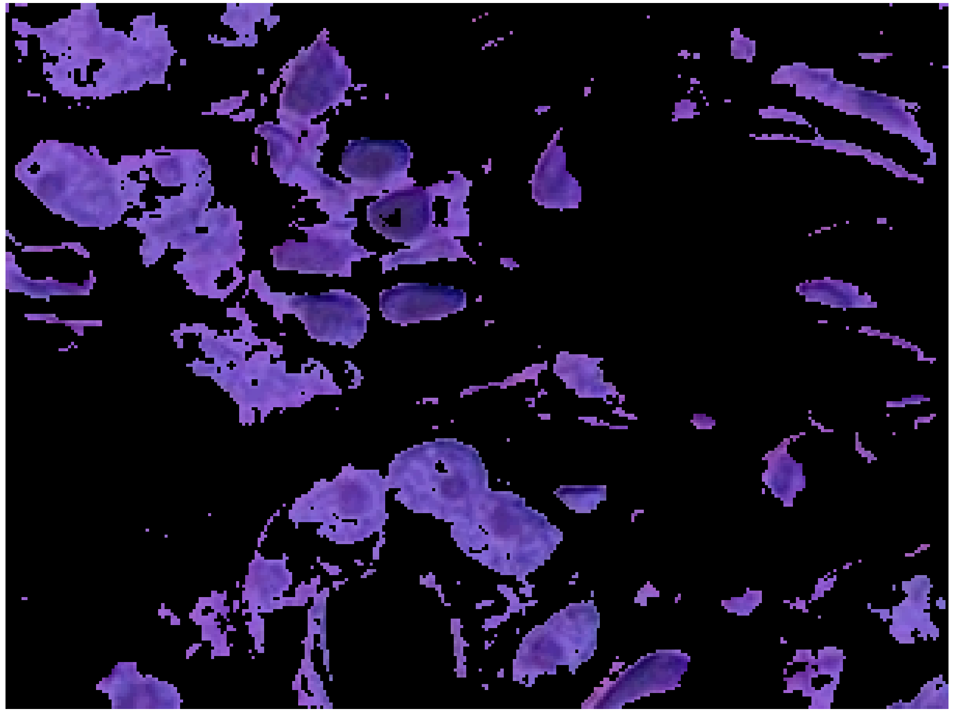
# Application

- Colour-Based Image Segmentation Using *K*-means

**Step 6**: Segment the nuclei into a separate image with the L* feature

- In cluster 1, there are dark and light blue objects (pixels). The dark blue objects (pixels) correspond to nuclei (with the domain knowledge).
- L* feature specifies the brightness values of each colour.
- With a threshold for L*, we achieve an image containing the nuclei only.

blue nuclei



# Summary

- *K*-means algorithm is a simple yet popular method for clustering analysis
- Its performance is determined by initialisation and appropriate distance measure
- There are several variants of *K*-means to overcome its weaknesses
  - *K*-Medoids: resistance to noise and/or outliers
  - *K*-Modes: extension to categorical data clustering analysis
  - CLARA: extension to deal with large data sets
  - Mixture models (EM algorithm): handling uncertainty of clusters

**Online tutorial**: how to use the *K*-means function in Matlab

https://www.youtube.com/watch?v=aYzjenNNOcc