Lecture 20
Unsupervised Clustering
ECEN 5283 Computer Vision

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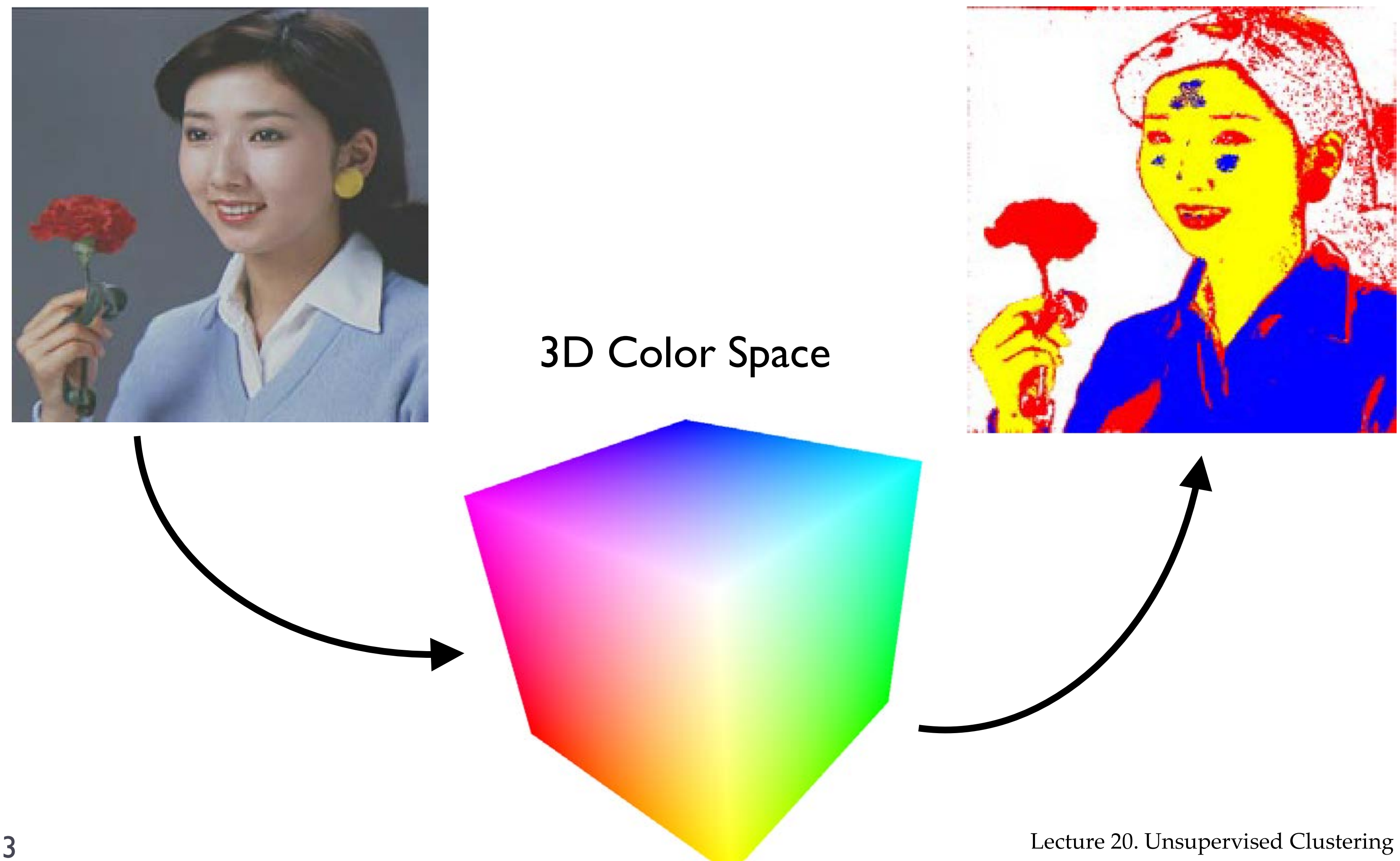
Goals

- To group a data set into different clusters.
- To study a few issues related to unsupervised clustering.
- To introduce the K-means clustering method.

Clustering in the Feature Space



Problem Formulation of Unsupervised Clustering

- Given a set of unlabelled data samples $\mathbf{D} = \{y_1, y_2, \ldots, y_n\}$ in a d-dimensional space, we partition the set D into a number of disjoint subsets

$$\mathbf{D} = \bigcup_{j=1}^{K} D_j, \quad D_i \bigcap D_j = \phi, i \neq j$$

So that points in each subset are coherent according to certain criterion denoted by *f(.)*. We denote a partition by

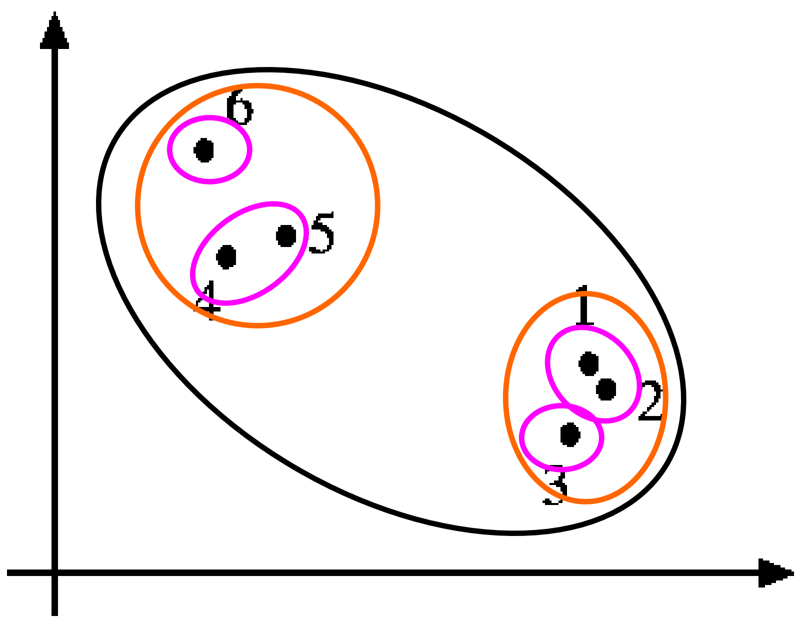
$$\Pi = \begin{pmatrix} D_1 & D_2 & \ldots & D_K \end{pmatrix}$$

Thus the problem is formulated as

$$\Pi^* = \arg_{\Pi} \max \boldsymbol{f}(\Pi).$$

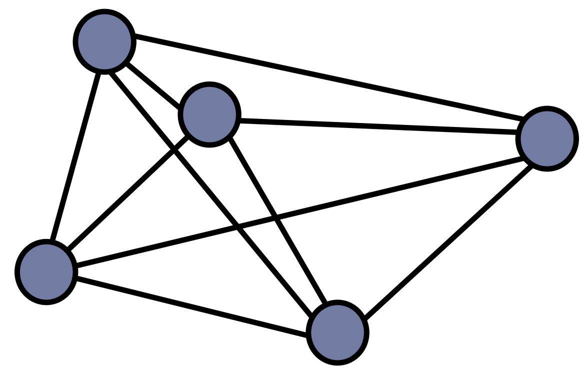
Two Problems to Avoid for Clustering

- There are two problems to avoid during clustering:
  - Under-fitting
  - Over-fitting



Two Issues to Consider for Clustering

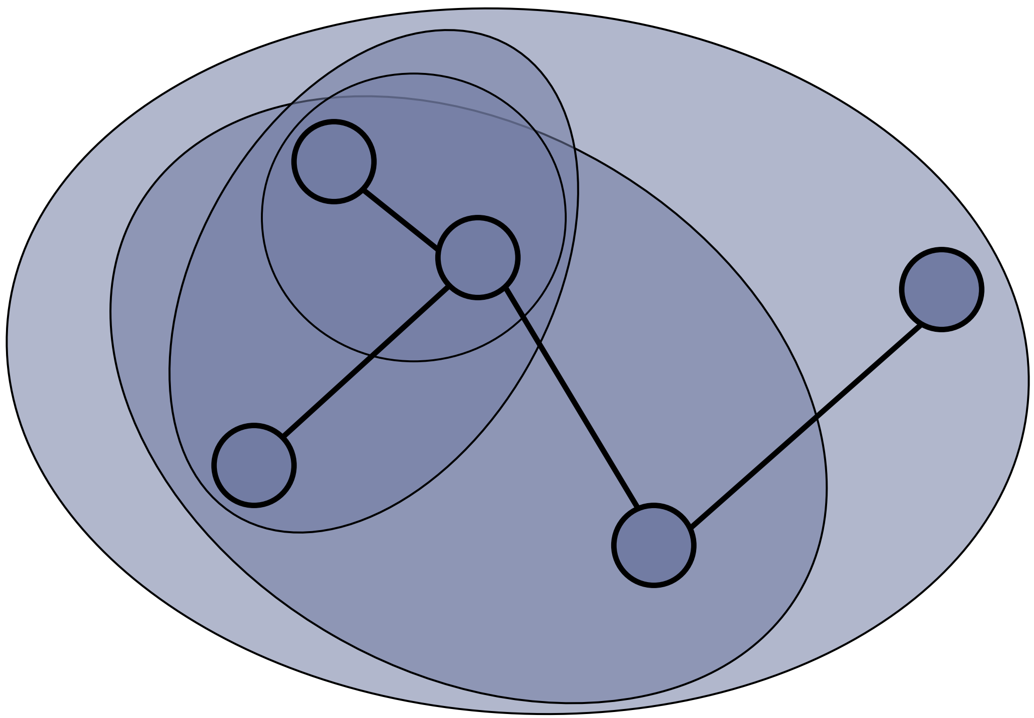
- There are two major issues in thinking of clustering:
  - What is a good distance metric?
    - Between two samples
    - Between a cluster and a sample
    - Between two clusters
  - How many clusters are there?



- There are two fashions of clustering
  - Agglomerative
    - From many to a few
  - Divisive
    - From one to a few

Agglomerative Clustering

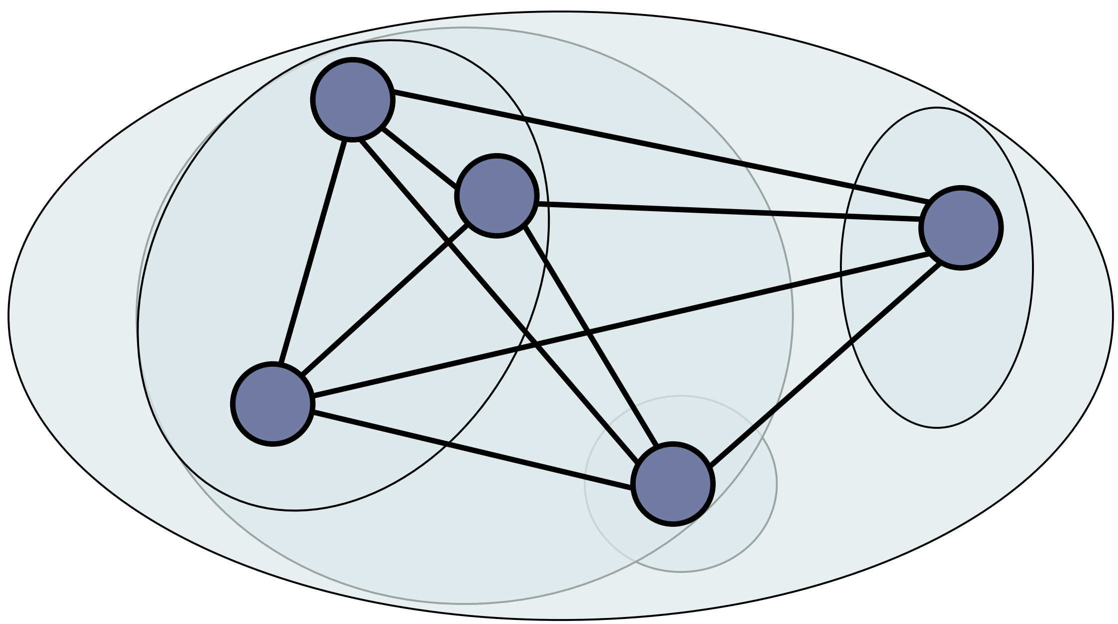
- Each object is initially placed into its own group. Each group contains only one object. Before we start the clustering, we need to decide on a threshold distance.



http://fconyx.ncifcrf.gov/~lukeb/agclout.html

Divisive Clustering (Cont'd)

- Divisive Clustering starts by placing all objects into a single group. Before we start the procedure, we need to decide on a threshold distance.



http://fconyx.ncifcrf.gov/~lukeb/diclust.html

K-means Clustering (Hard K-mean)

- Goal: Given the number of classes k, we attempt to optimize an objective function.
- Objective:
  - We want to segment data points in the feature space, then **y** represent the feature vector, and **c** is the center of a cluster.
  - We assume that elements are close to center of their cluster, yielding the objective function (intra-class divergence)

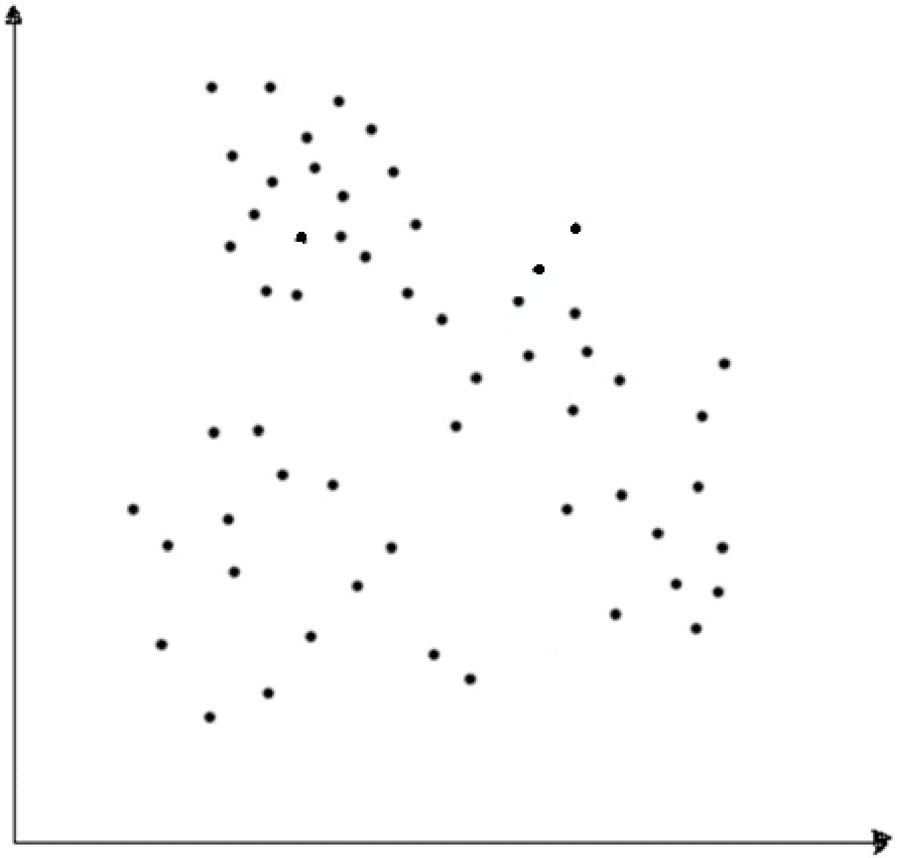
$$\Phi(\text{clusters}, \text{data}) = \sum_{i \in \text{clusters}} \left\{ \sum_{j \in i^{th} \text{ cluster}} \left| \mathbf{y}_j - \mathbf{c}_i \right|^2 \right\}$$

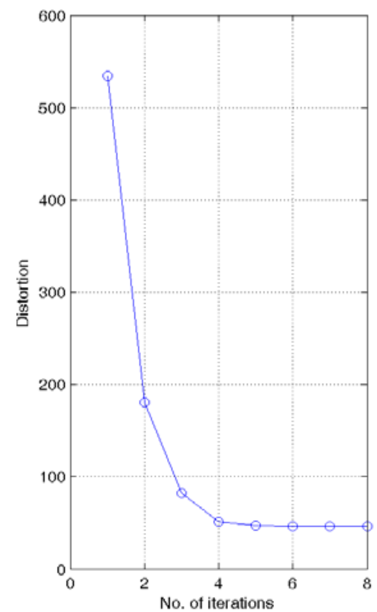
- Two activities:
  - Assume the cluster centers are known, and allocate each data point to the closest cluster center.
  - Assume the allocation is known, and compute a new set of cluster centers. Each center is the mean of the points allocated to that cluster.

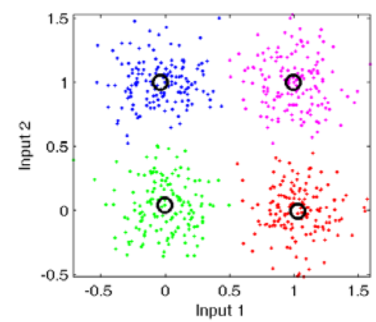
K-means Algorithm

- Form K-means clusters from a set of n-dimensional vectors.
  - Set *Nc* =1 (iteration number).
  - Choose randomly a set of K means, $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_k\}$.
  - For each vector y, compute $D(\mathbf{y}, \mathbf{c}_k)$ for each *k*=1,2,…,*K*, and assign y to the cluster with the nearest distance.
  - Increment *Nc* by 1 and update the means based on new class labels to get a new set of centers $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_k\}$.
  - Repeat until no change to $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_k\}$ or the objective function has insignificant change, or *Nc*=*Nmax*
- This process eventually converges to a local minimum of the objective function.

K-means Clustering Examples







K-means Clustering for Color Quantization

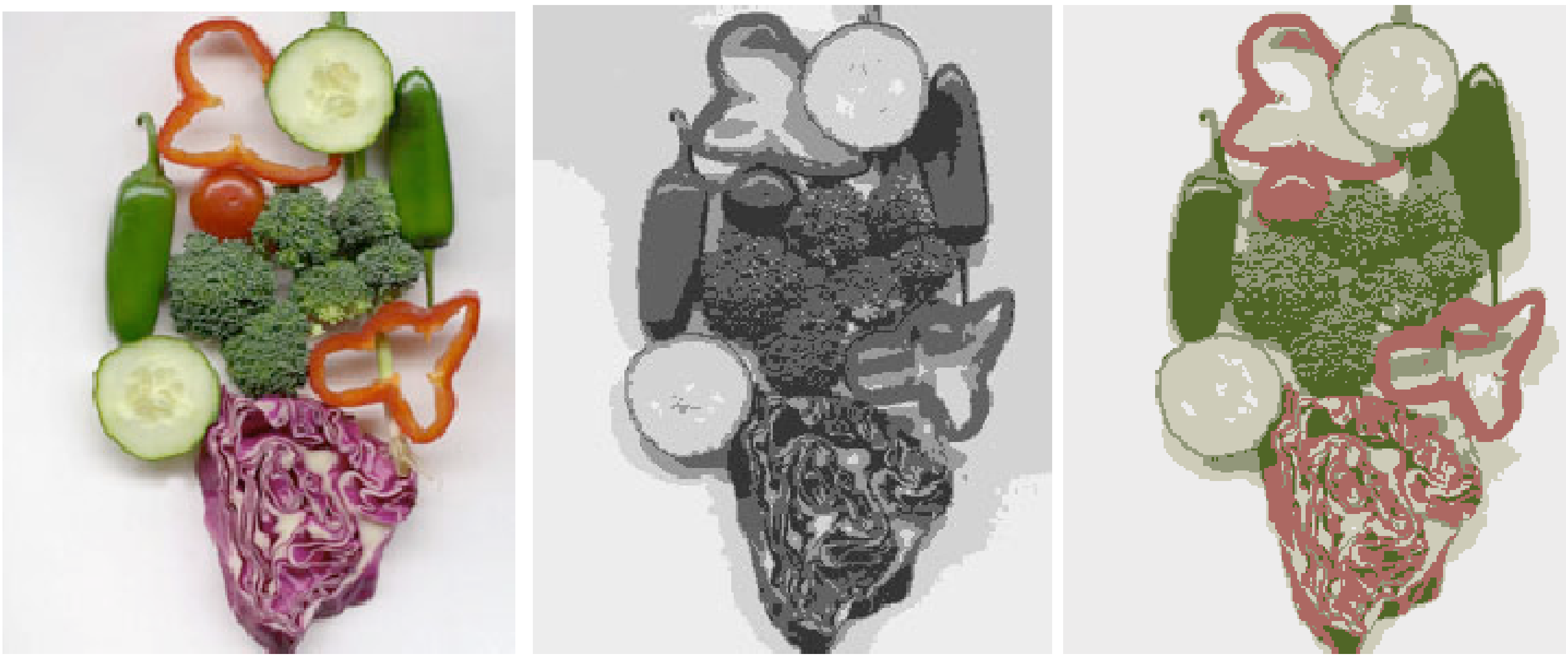
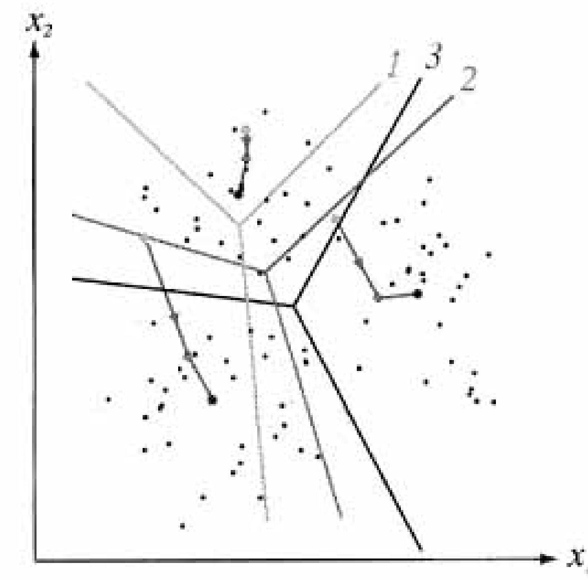


Figure 16.13. On the left, an image of mixed vegetables, which is segmented using k-means to produce the images at center and on the right. We have replaced each pixel with the mean value of its cluster; the result is somewhat like an adaptive requantization, as one would expect. In the center, a segmentation obtained using only the intensity information. At the right, a segmentation obtained using colour information. Each segmentation assumes five clusters.

Why K-means Converge?

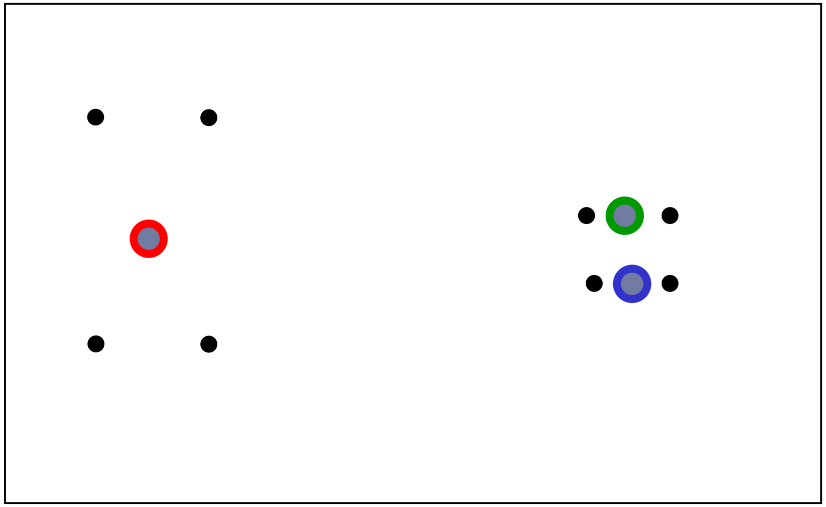
- Whenever an assignment is changed, the sum squared distances of data-points from their assigned cluster centers is reduced.
- Whenever a cluster center is moved the sum squared distances of the data-points from their currently assigned cluster centers is reduced.
- If the assignments do not change in the assignment step, we have converged.



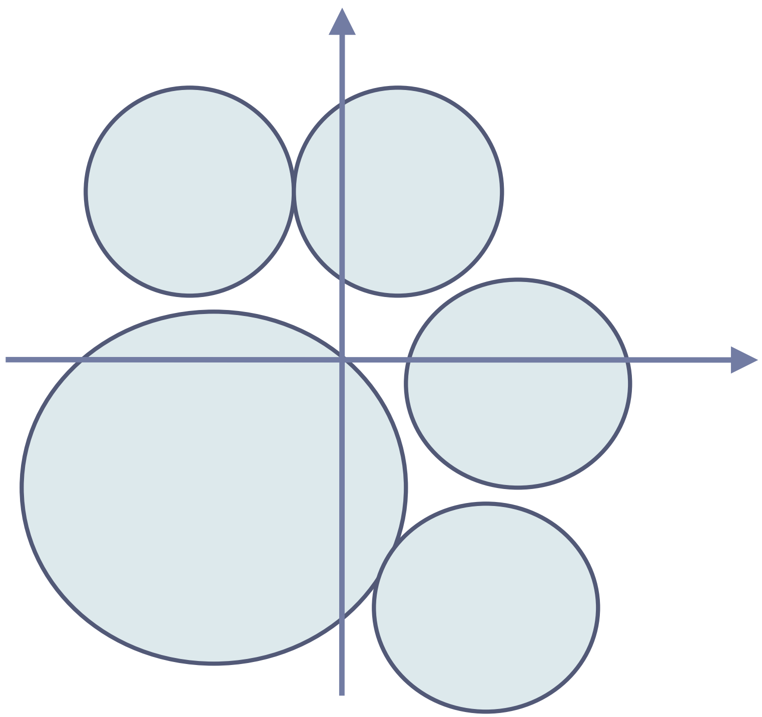
Why K-means can be stuck at a local minima?

- There is nothing to prevent k-means getting stuck at local minima.
- We could try many random starting points
- We could try non-local split-and-merge moves: Simultaneously merge two nearby clusters and split a big cluster into two.

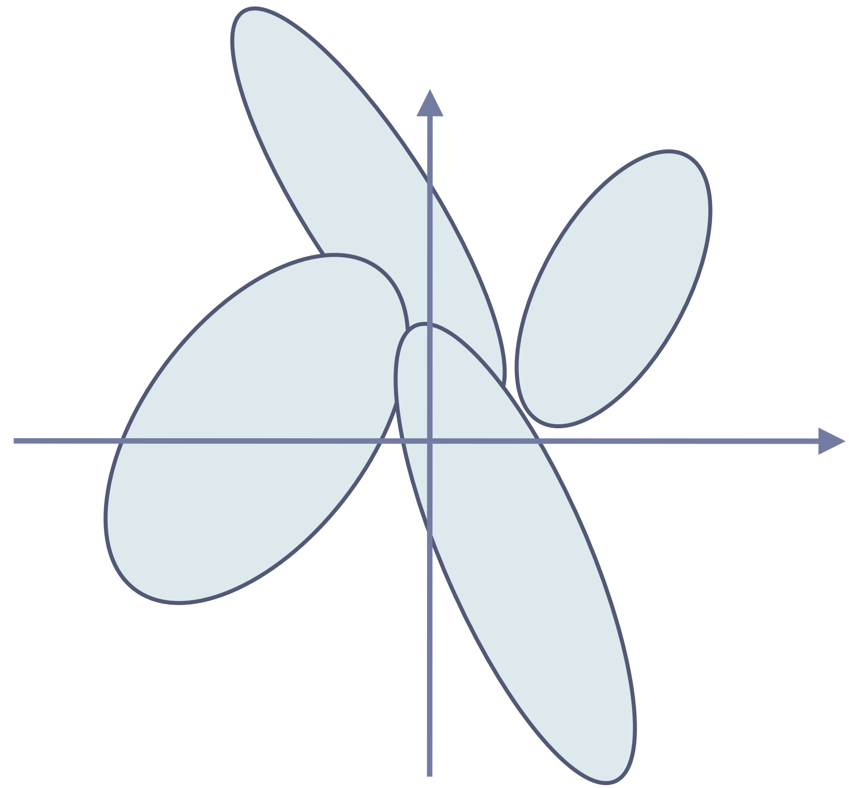
A bad local optimum



Underlying Assumption of K-means



All feature distributions are isotropic



K-mean does not work for the case of non-isotropic feature distributions