

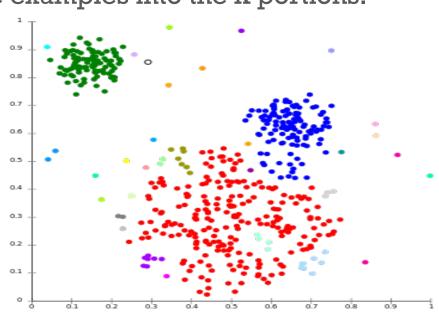
#### Clustering Algorithms

K-means
Gaussian Mixture Model



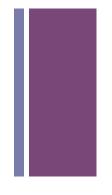
## Clustering

- Kind of Unsupervised Learning problem
- Given: N unlabelled examples:  $\{x_1, \ldots, x_N\}$ , each with D dimensions (features):  $\{f_1, \ldots, f_D\}$ , Number of clusters K
- Target: how to group all the examples into the K portions.
- Example:
  - K-means
  - Gaussian Mixture Model









- Nonprobabilistic technique
- Hard assignment : each example must belongs to one cluster
- Cluster a group of data points whose inter-point distances are small compared with the distances to points outside of the cluster.

## \*K-mean Algorithm

#### ■ Given

- X data set  $\{x_1, ..., x_N\}$  consisting of N observations of a random D-dimensional Euclidean variable x.
- Goal is to partition the data set into some number K of clusters

#### Define

• set of D-dimensional vectors  $\mu_k$ , where k = 1, ..., K, in which  $\mu_k$  is a prototype associated with the  $k^{th}$  cluster.

#### ■ Goal:

- find an assignment of data points to clusters
- such that the sum of the squares of the distances of each data point to its closest vector  $\mu_k$ , is a minimum.

## K-mean (Objective Function)

- For each data point  $x_n$ , we introduce a corresponding set of binary indicator variables  $\mathbf{r}_n^{\ k} \in \{0,1\}$ , where  $k=1,\ldots,K$  describing which of the K clusters the data point  $x_n$  is assigned to
- objective function, sometimes called a *distortion measure*,

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

■ Goal: find values for the  $\{r_n^k\}$  and the  $\{\mu_k,\}$  to minimize J

## K mean algorithm



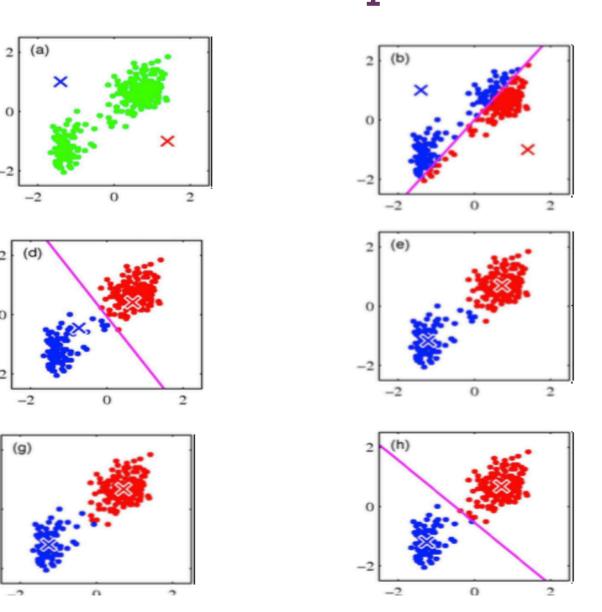
$$\mu^{(0)} = \mu_1^{(0)}, \dots, \mu_k^{(0)}$$

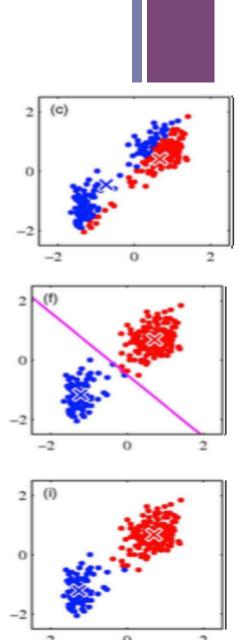
■ Assignment step: Assign each point  $i \in \{1,...m\}$  to nearest center:  $C^{(t)}(j) \leftarrow \arg\min_i ||\mu_i - x_j||^2$ 

■ **Update step**:  $\mu_i$  becomes centroid of its point:

$$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C(j)=i} ||\mu - x_j||^2$$

## K-mean Example





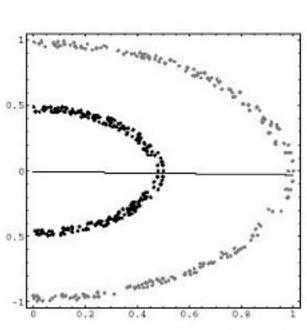




- Fast, robust and easier to understand.
- Relatively efficient: O(tknd), where n is # objects, k is # clusters, d is # dimension of each object, and t is # iterations. Normally, k, t, d << n.
- Gives best result when data set are distinct or well separated from each other.

### Limitation

- Makes hard assignments of points to clusters
  A point either totally belongs to a cluster or not at all  $\frac{1}{0}$  0.5 1
- No notion of a soft/fractional assignment (i.e., probability of being assigned to each cluster: say K = 3 and for some point  $x_n$ , p1 = 0.7, p2 = 0.2, p3 = 0.1)
- K-means often doesn't work when clusters are not round shaped, and/or may overlap, and/or are unequal
- Unable to handle nonlinear or noisy data and outliers.



(a)

0.5

#### + K mean DEMO







## Soft Assignment

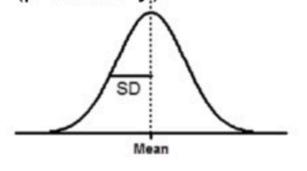
#### ■ K-means algorithm:

- every data point is assigned uniquely to one, and only one, of the clusters.
- Some data points that lie roughly midway between cluster centers.
- **Solution**: adopting a probabilistic approach, we obtain '**soft**' assignments of data points to clusters in a way that reflects the level of uncertainty over the most appropriate assignment.

## Gaussian Mixture Model GMM

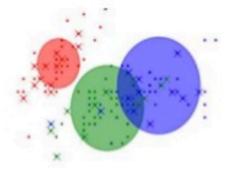
#### Gaussian

"Gaussian is a characteristic symmetric "bell curve" shape that quickly falls off towards 0 (practically)"



#### Mixture Model

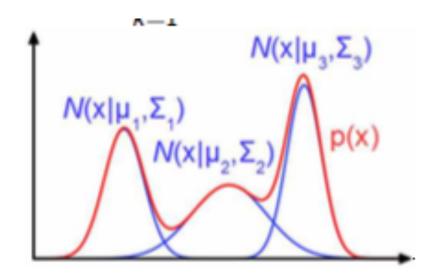
"mixture model is a probabilistic model which assumes the underlying data to belong to a mixture distribution"





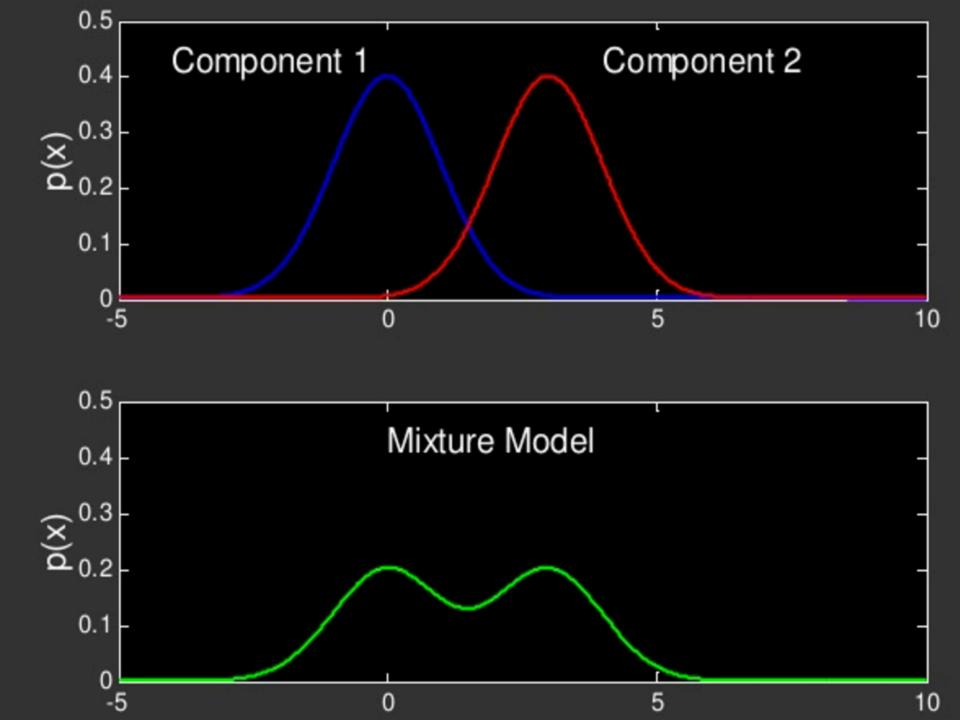
## Gaussian Mixture Model GMM

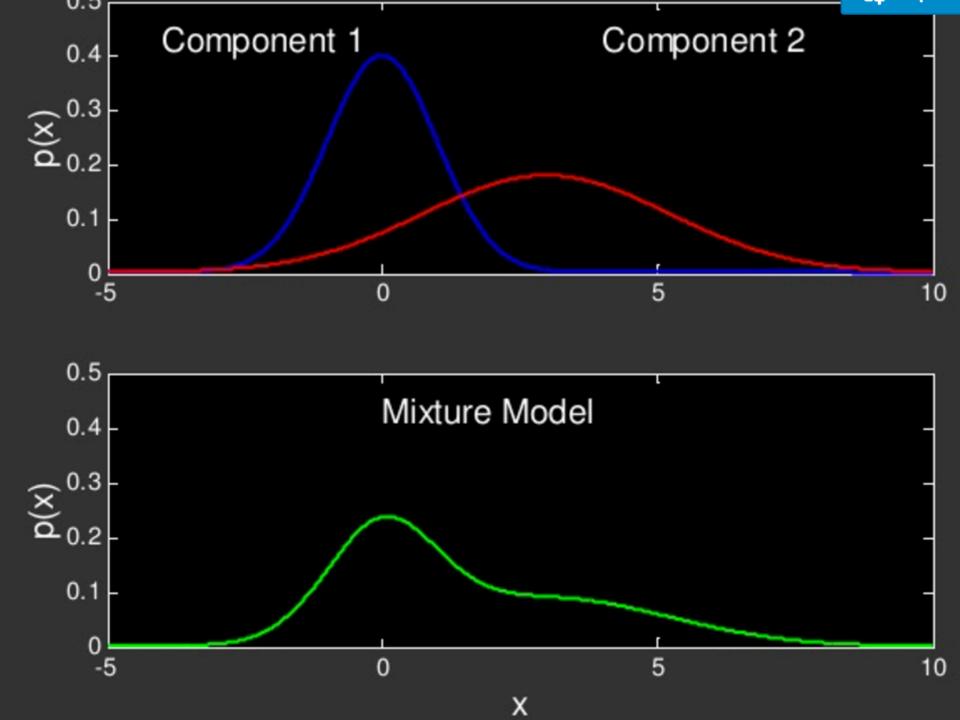
- Gaussian (normal) distribution: model for the distribution of continuous variables
- **Mixture Distribution**: probability distribution of a random variable that is derived from a collection of other random variable.
- A **probability density p**(x) represents a mixture distribution or mixture model

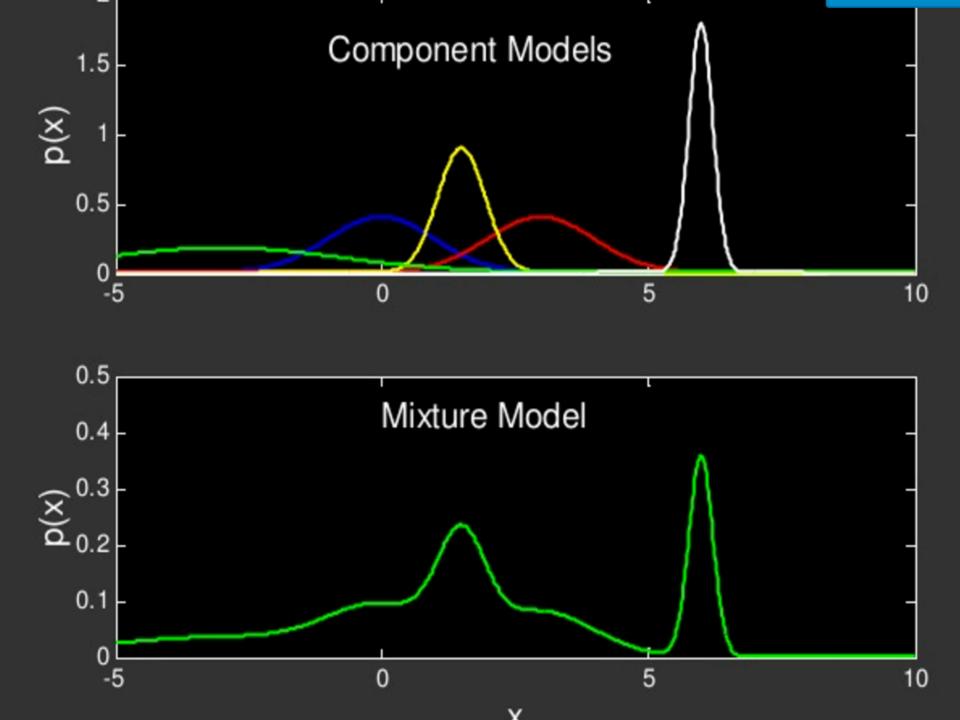


### Gaussian Mixture Model GMM

■A Gaussian mixture model is a probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters.





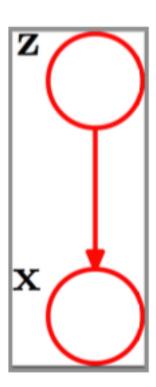


# Gaussian Mixture Model: Joint Distribution



$$p(x,z) = p(z)p(x \mid z) = \pi_z N(x \mid \mu_z, \Sigma_z)$$

- $\blacksquare$   $\Pi_z$  is probability of choosing cluster z.
- X | Z = z has distribution N( $\mu_z$ ,  $\Sigma_z$ ).



## Learning the Gaussian Mixture Model - likelihood function

■ we only observe X, we need the **marginal distribution**:

$$p(x) = \sum_{z=1}^{k} p(x,z)$$
$$= \sum_{z=1}^{k} \pi_z \mathcal{N}(x \mid \mu_z, \Sigma_z)$$

## Learning the Gaussian Mixture Model - likelihood function

■ The model **likelihood** for  $D = \{x_1,...,x_n\}$  is

$$L(\pi, \mu, \Sigma) = \prod_{i=1}^{n} p(x_i)$$

$$= \prod_{i=1}^{n} \sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z)$$

■ As usual, we'll take **objective function** to be the log of this:

$$J(\pi, \mu, \Sigma) = \sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \pi_{z} \mathcal{N}(x_{i} \mid \mu_{z}, \Sigma_{z}) \right\}$$



## Gaussian Mixture Model: Conditional Distribution

■ We observe X = x, the **conditional distribution** of the cluster Z given X = x is

$$p(z \mid X = x) = p(x,z)/p(x)$$

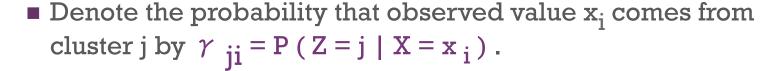
- The conditional distribution is a **soft assignm**ent to clusters.
- $z \in \{1,...,k\}$ , Cluster assignment Z is called a **hidden** variable

## Learning the Gaussian Mixture Model

#### ■ Build GMM

- 1. Cluster probabilities  $\Pi = (\Pi_1, ..., \Pi_k)$
- 2. Cluster means  $\mu = (\mu_1, ..., \mu_k)$
- 3. Cluster covariance matrices:  $\Sigma = (\Sigma_1, ..., \Sigma_k)$
- We have a probability model: let's find the MLE.
- Suppose we have data  $D = \{x_1,...,x_n\}$ . We need the **model likelihood** for D.

## Learning the Gaussian Mixture Model



- The responsibility that cluster j takes for observation xi. Computationally,
  - $P_{ji} = P(Z = j \mid X = x_i)$
  - $\gamma_{ji} = p(Z=j, X=x_i)/p(x) = \pi_j N(xi \mid \mu j, \Sigma j)/p(x)$
- The vector  $\gamma_1,...,\gamma_k$  is exactly the soft assignment for  $x_i$ .

## Exception Maximization Learning

- 1. Initialize parameters  $\mu$ , π,  $\Sigma$ .
- 2. "E step". Evaluate the responsibilities using current parameters  $\pi: \mathcal{N}(\mathbf{x}; | \mathbf{u}; \Sigma_i)$

$$\gamma_i^j = \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_{c=1}^k \pi_c \mathcal{N}(x_i \mid \mu_c, \Sigma_c)},$$

- for i = 1,...,n and j = 1,...,k.
- 3. "M step". Re-estimate the parameters using responsibilities  $\frac{n}{1}$

$$\mu_c^{\text{new}} = \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c x_i$$

$$\Sigma_c^{\text{new}} = \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c (x_i - \mu_{\text{MLE}}) (x_i - \mu_{\text{MLE}})^T$$

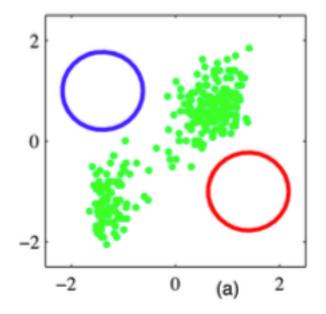
$$\pi_c^{\text{new}} = \frac{n_c}{n_c},$$

4. Repeat from Step 2, until log-likelihood converges.

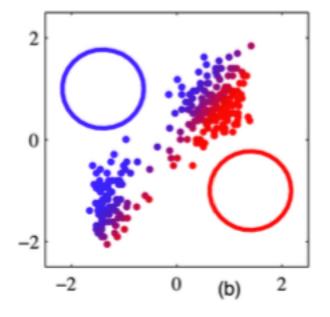


## **EM Example**

#### 1. Initialization

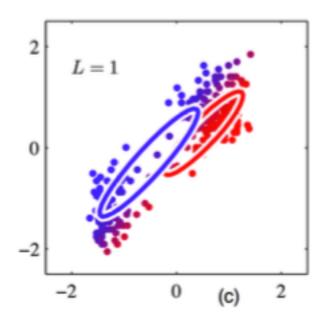


#### 2. First soft assignment

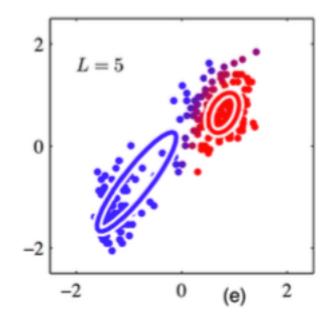


## EM Example

#### 3. Updating Parameters:



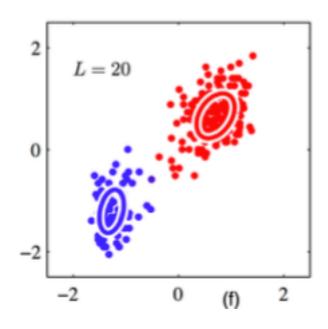
#### 4. Repeat Assignment





## EM Example







### Advantages/Dis of GMM

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#### Strength

- √ GMM model accommodates mixed membership
- √ Flexible in terms of cluster covariance

#### Weakness:

- X Computationally expensive if the number of distribution is large, or the data set contains very few observed data points
- X Hard to estimate number of clusters



https://lovasoa.github.io/expectation-maximization/dist/



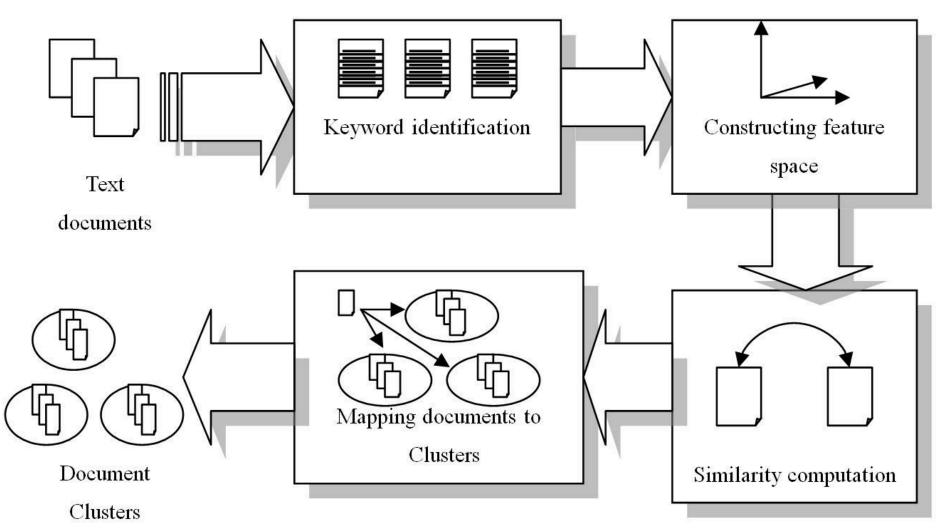


## Clustering-NLP example

- Document clustering
  - The similarity measure is the key point to the clustering problem.
  - represent each document as an array of numbers Using VSM
    - Count up the number of times each word appears in the document.
    - Choose a set of "feature" words that will be included in your vector. This should exclude extremely common words ("stopwords") like "the", "a", etc.
    - Make a vector for each document based on the counts (.TF X IDF) of the feature words.
  - Apply k-means, EM to cluster documents by maximizing the likelihood of the unlabeled documents









## Clusetring related documents

#### [PDF] A survey on various approaches in dogument clustering

..., V Preamsudha, MP **Scholar** - International ..., 2017 - pdfs.semanticscholar.org
Abstract Document clustering is the process of segmenting a particular collection of texts into subgroups including content based similar ones. The purpose of document clustering is to meet human interests in information searching and understanding. Nowadays all paper
Cited by 15 Related articles All 3 versions Cite Save More

## A new unsupervised method for **document clustering** by using WordNet lexical and conceptual relations

DR Recupero - Information Retrieval, 2007 - Springer

... improve the preprocessing since it is the most critical step for the generation of an appropriate document representation. The other one is how the use of WordNet benefits the cluster labeling task: having documents represented by concepts ... Frequent term-based text clustering. ...

Cited by 66 Related articles All 7 versions Web of Science: 16 Cite Save

#### Ant-based and swarm-based clustering

J Handl, B Meyer - Swarm Intelligence, 2007 - Springer

... Homogeneous ants for web **document** similarity modeling and categorization. ... A stochastic heuristic for visualising graph **clusters** in a bi-dimensional space prior to partitioning. Journal of Heuristics, 5(3), 327–351. ... Antclust: ant **clustering** and web usage mining. ... Cited by 134 Related articles. All 5 versions. Cite. Save

## NLP example

- D1: there is a dog who chased a cat
- D2: someone ate pizza for lunch
- D3: the dog and a cat walk down the street toward another dog
- **feature words** are [dog, cat, street, pizza, lunch]
- [1, 1, 0, 0, 0] // dog l time, cat l time
- [0, 0, 0, 1, 1] // pizza 1 time, lunch 1 time
- [2, 1, 1, 0, 0] // dog 2 times, cat 1 time, street 1 time
- Apply Clustering Algorithm Cosine similarity between vectors



# Document clustering using K-means

- Assuming we have data with no labels for news and technical data
- We want to be able to categorize a new document into **one** of the 2 classes (K=2)
- We can extract represent document as feature vectors
  - Features can be word id or other NLP features such as POS tags, word context etc (D=total dimension of Feature vectors)
  - N documents are available
- Randomly initialize 2 class means
- $\blacksquare$  Compute square distance of each point (x\_n)(D) to class means (  $\mu$   $_k$ )
- Assign the point to K for which  $\mu_k$  is lowest
- lacktriangle Re-compute  $\mu$  and re-iterate until converge

#### References

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- 8. Kaur, R., & Kaur, A. (2016). Text Document Clustering and Classification using K-Means Algorithm and Neural Networks. *Indian Journal of Science and Technology*, 9(40).
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