Lecture 12
Clustering, K-Means and EM

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING

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Outline

- ❑Motivating Example: Document clustering
- ❑K-means
- ❑K-means for document clustering
- ❑Latent semantic analysis (Review of PCA)
- ❑Gaussian Mixture models (GMMs)
- ❑Expectation Maximization (EM) fitting of GMMs
- ❑Clustering for image processing

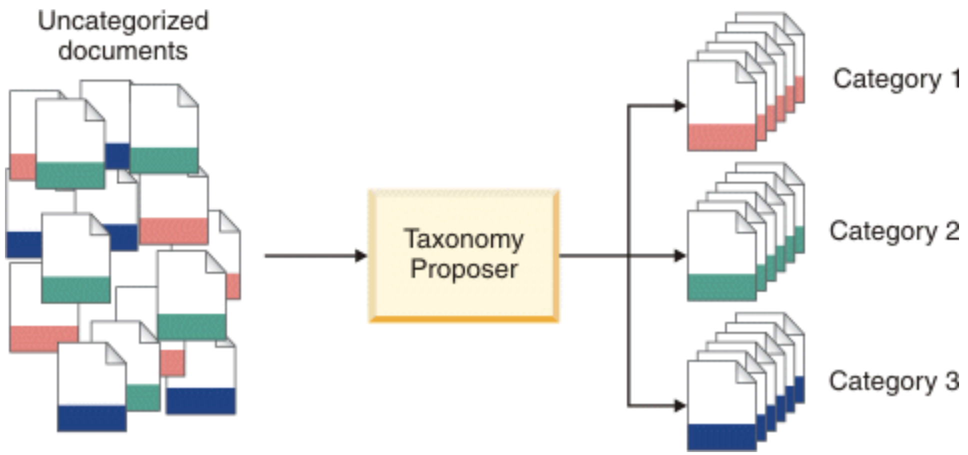
Document Clustering

IBM

IBM Knowledge Center

Content Classification > Content Classification 8.8.0 > Configuring > Cat
Using the Taxonomy Proposer to discover new categories

Using the Taxonomy Proposer to discover new categories

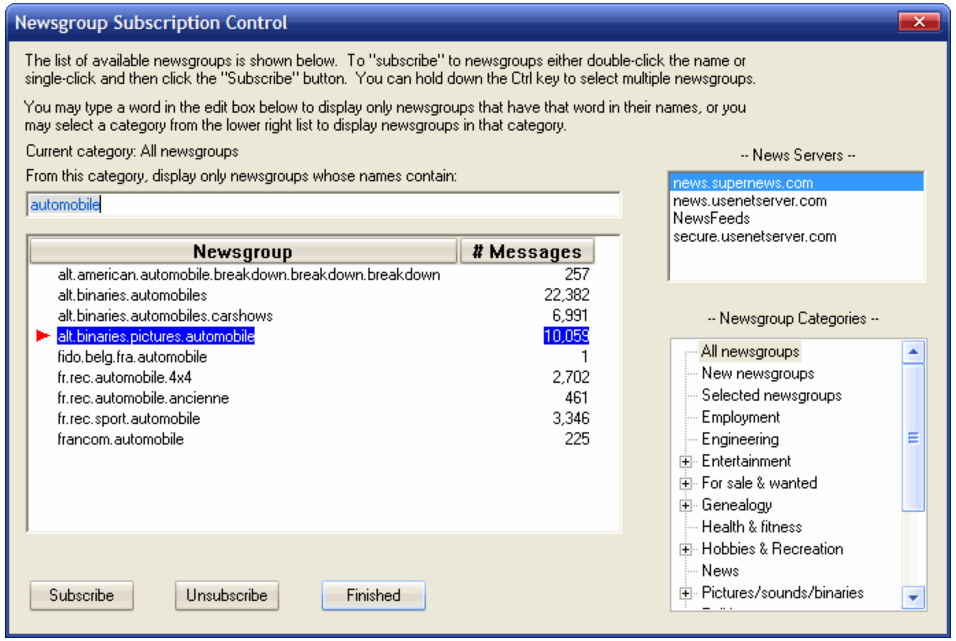


- Data mining
- Often have huge numbers of documents
- How can we organize this?

- Key idea: documents are often in clusters

- Can we detect these clusters?
- Can be a lucrative service
  - See IBM service to left

UseNet Newsgroups



- Began in late 1970s
- Discussion groups for various topics
  - Started on early university networks
  - Migrated to Internet
  - Peaked in 1990s
- Useful for studying clustering
  - Simple documents
  - “ground truth”: Docs have categories

Loading the Data

- See demo_doc_cluster.ipynb
- Taken from http://scikit-learn.org/stable/auto_examples/text/document_clustering.html
- Newsgroups built into sklearn

```
categories = [
    'alt.atheism',
    'talk.religion.misc',
    'comp.graphics',
    'sci.space',
]
# Uncomment the following to do the analysis on all the categories
#categories = None

print("Loading 20 newsgroups dataset for categories:")
print(categories)

dataset = fetch_20newsgroups(subset='all', categories=categories,
                             shuffle=True, random_state=42)
```

```
Loading 20 newsgroups dataset for categories:
['alt.atheism', 'talk.religion.misc', 'comp.graphics', 'sci.space']
```

A Typical Newsgroup Post

```
ind = 10
data_ex = dataset.data[ind]
cat_ex  = dataset.target_names[labels[ind]]
print('Post from {0:s}'.format(cat_ex))
print()
print(data_ex)
```

```
Post from comp.graphics

From: richter@fossi.hab-weimar.de (Axel Richter)
Subject: True Color Display in POV
Keywords: POV, Raytracing
Nntp-Posting-Host: fossi.hab-weimar.de
Organization: Hochschule fuer Architektur und Bauwesen Weimar, Germany
Lines: 6


Hallo POV-Renderers !
I've got a BocaX3 Card. Now I try to get POV displaying True Colors
while rendering. I've tried most of the options and UNIVESA-Driver
but what happens isn't correct.
Can anybody help me ?
```

- Data for the posts are in:
  - Dataset.data
  - Dataset.labels
  - Dataset.target_names

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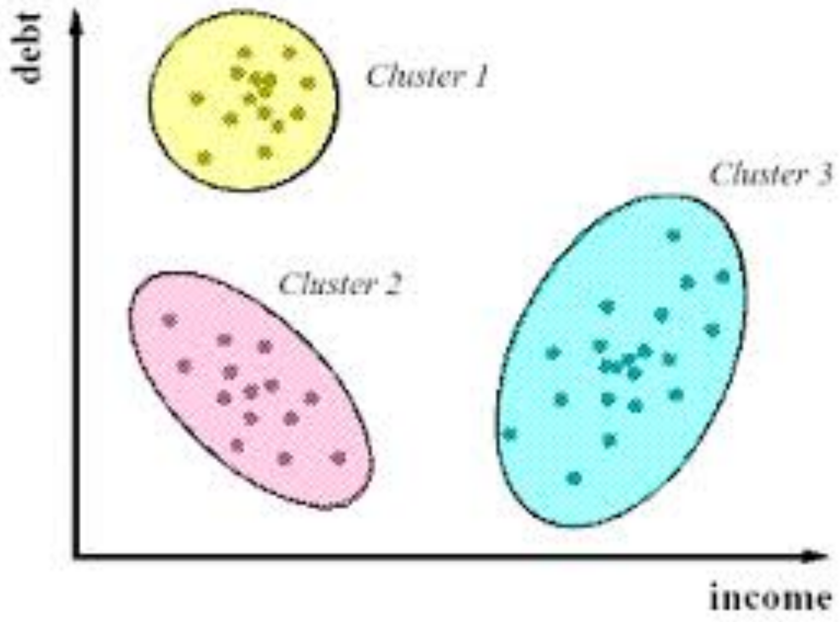
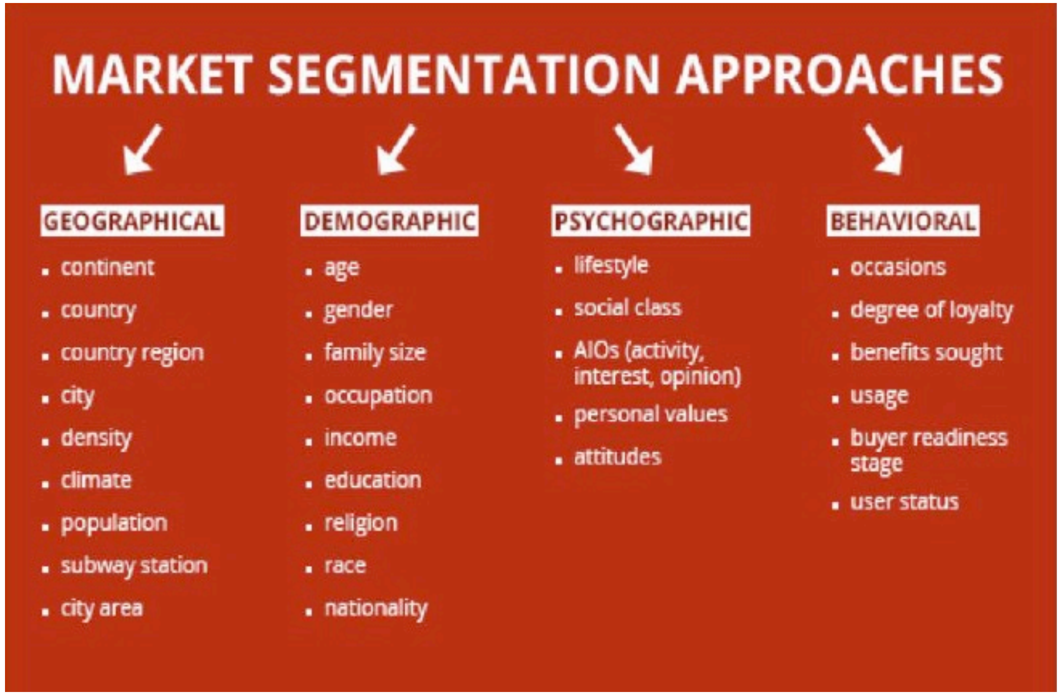
Clustering

- Given $N \times d$ data matrix: $\boldsymbol{X}$
  - Each row is one sample, x_n
- Problem: Group data into K clusters
- Mathematically:
  - Assign each sample to a cluster
  - Assign $\sigma_n \in \{1, \ldots, K\}$: Cluster label for each sample
- Want samples in same cluster to be "close"
  - $\|x_n - x_m\|$ is small when $\sigma_n = \sigma_m$



Clustering

- Clustering has many applications
  - Any time you want to segment data
  - Uncovering latent discrete variables
- Examples:
  - Segmenting sections of an image
  - Segmenting customers in market data

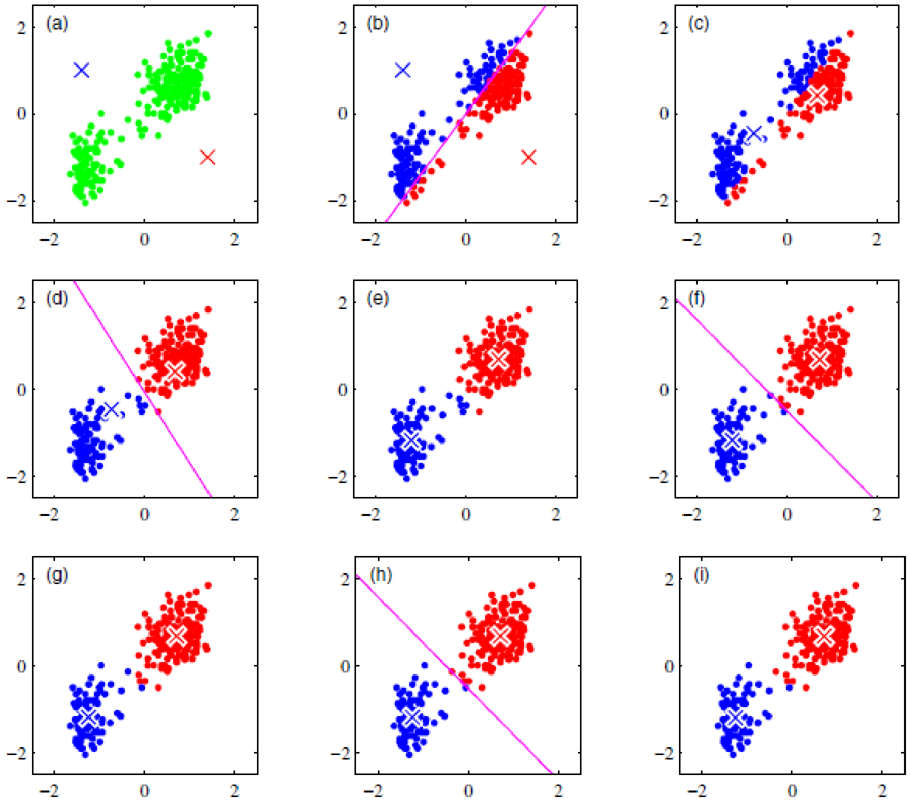


From: Market segmentation possibilities in the tourism market context of South Africa

K-means

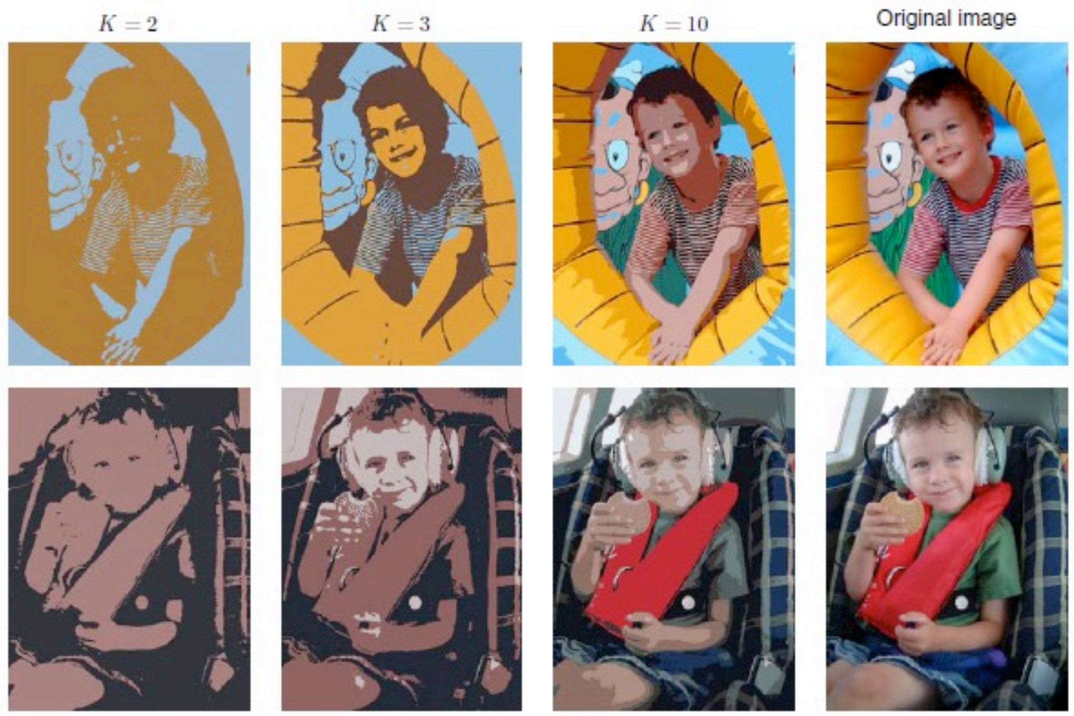
- A simple iterative algorithm to determine:
  - μ_i = mean of each cluster (hence, the name K-means)
  - $\sigma_n \in \{1, \ldots K\}$ = cluster that data point x_n belongs to
  - Minimize: $J = \sum_{i=1}^{K} \sum_{n \in C_i} \|x_n - \mu_i\|^2$ (MSE of all samples in C_i from its center)
- Step 0: Start with guess at σ_n or μ_i
- Step 1: Update mean of each cluster: μ_i = average of x_n in C_i (centroid rule)
- Step 2: Update cluster membership: $\sigma_n = \arg\min_i \|x_n - \mu_i\|^2$ (nearest neighbor rule)
- Return to step 1

K-Means illustrated



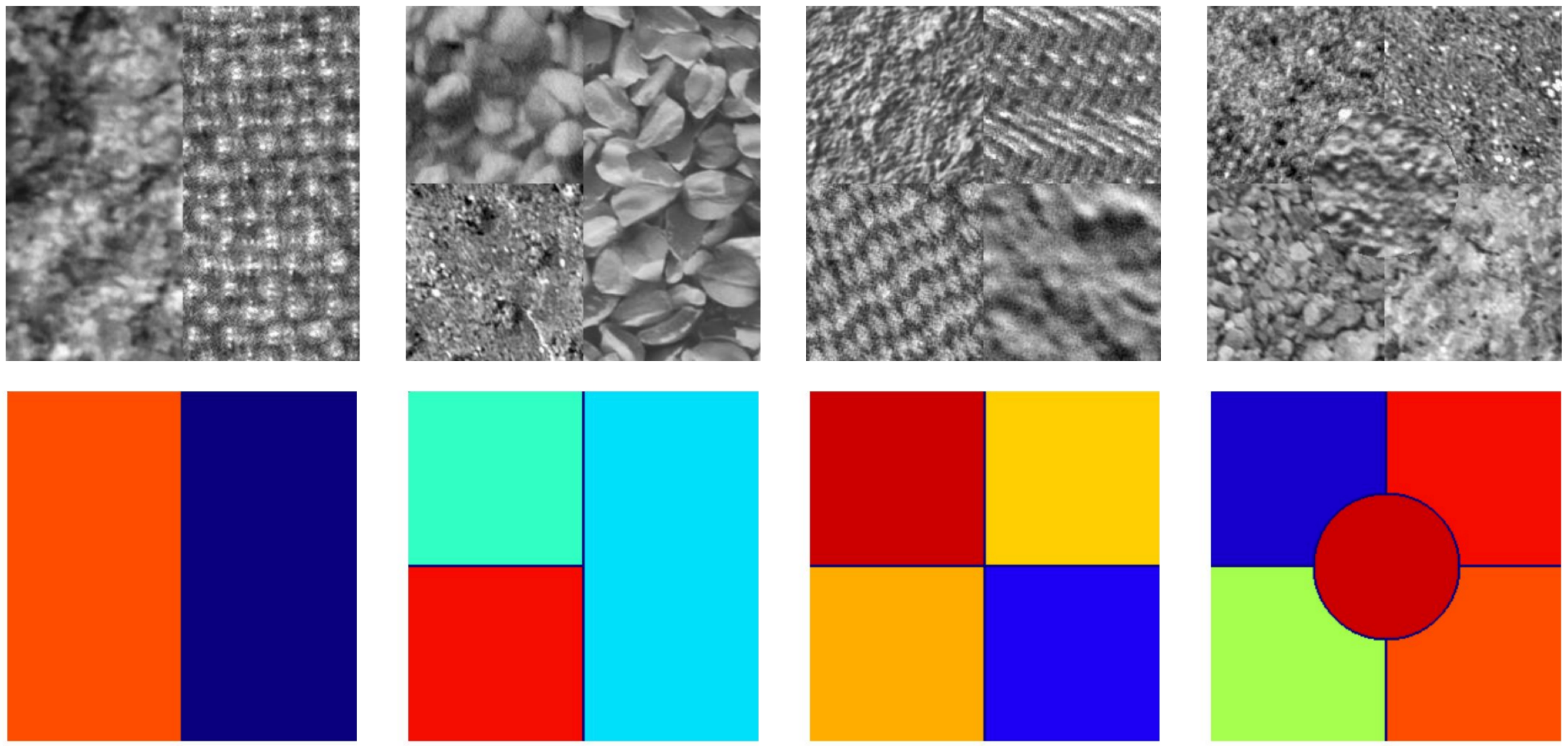
- From Bishop, Chapter 9.
- K-Means on “old faithful” data set

Image Segmentation Based on Color



- Also from Bishop.
- Use K-means on the RGB values (dimension = 3)

Image segmentation based on texture



Texture at each pixel is usually described by some statistics of the neighborhood surrounding the pixel.

Convergence

- Will always converge to a "local" minima of cost function

$$J = \sum_{i=1}^{K} \sum_{n=1}^{N} r_{ni} \|x_n - \mu_i\|^2$$

  - Subject to $r_{ni} = 0$ or 1 and $\sum_i r_{ni} = 1$

- K-means alternately decreases J
  - Proof on board

- But, can get stuck in a local minima
  - May need good selection of initial condition

Distance measures

- Distance measures
  - How to measure similarity between samples?
  - Above algorithms used squared distance $||x_n - x_m||$

- Many possibilities
  - What features to use?
  - Should you normalize entries?
  - What distance metric should you use?

Initialization

- Initialization:
  - Final limit of K-means depends on initial condition
  - May obtain poor clustering with bad initial condition
- Possible solutions:
  - K-means++: http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf
  - Provides good initial condition based on data
  - Multiple initial starts

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Bag of Words

Document 1

The quick brown fox jumped over the lazy dog's back.

Document 2

Now is the time for all good men to come to the aid of their party.

Term	Document 1	Document 2
aid	0	1
all	0	1
back	1	0
brown	1	0
come	0	1
dog	1	0
fox	1	0
good	0	1
jump	1	0
lazy	1	0
men	0	1
now	0	1
over	1	0
party	0	1
quick	1	0
their	0	1
time	0	1

Stopword List
for
is
of
the
to

- Document is natively text
- Must represent as a numeric vector
- Represent by word counts
  - Enumerate all words
  - Each document is count of frequencies
- Stopwords
  - Very common words
  - Not informative

Discussion Questions

- Is the absolute number of times a word appears the correct metric?

- What about the length of the document?
- What about the frequency of the word?
- What words “matter”?

Term Frequency – Inverse Document Frequency

- Use TF-IDF weight for vectors:

$$X[n,i] = \quad TF_{i,n} \quad \times \quad IDF_i$$

Document weight vector

Term frequency

$$= \frac{\text{num times word } i \text{ in doc } n}{\text{total num words in doc } n}$$

Inverse doc frequency

$$= \log\left[\frac{\text{Total num docs in corpus}}{\text{Num docs with word } i}\right]$$

Computing TF-IDF in Python

- Can compute the TF-IDF using sklearn functions

```
print("Extracting features from the training dataset using a sparse vectorizer")
t0 = time()
vectorizer = TfidfVectorizer(max_df=0.5, max_features=opts.n_features,
                             min_df=2, stop_words='english',
                             use_idf=opts.use_idf)
X = vectorizer.fit_transform(dataset.data)
print("done in %fs" % (time() - t0))
print("n_samples: %d, n_features: %d" % X.shape)
print()
```

```
Extracting features from the training dataset using a sparse vectorizer
done in 1.451549s
n_samples: 3387, n_features: 10000
```

Typical TF-IDF scores

weimar	0.565396
pov	0.518174
renderers	0.183033
univesa	0.178595
und	0.174842
fuer	0.171591
true	0.159214
raytracing	0.150534
displaying	0.140240
ve	0.139752
options	0.134309
rendering	0.133027
driver	0.129544
happens	0.122540
colors	0.119138
card	0.113776
display	0.108457
germany	0.108231
tried	0.106282
color	0.103717
anybody	0.100397
correct	0.100234
isn	0.084694
got	0.081865
keywords	0.081865
try	0.080601
help	0.078058
nntp	0.044277
host	0.043985
posting	0.042608

- Code to display terms with highest scores

```
xi = X[doc_ind,:].todense()
term_ind = xi.argsort()[:, ::-1]
xi_sort = xi[0,term_ind]
terms = vectorizer.get_feature_names()

for i in range(30):
    term = terms[term_ind[0,i]]
    tfidf = xi[0,term_ind[0,i]]
    print('{0:20s} {1:f} '.format(term, tfidf))
```

Running K-Means

- Use Python built-in function

```
km = KMeans(n_clusters=true_k, init='k-means++', max_iter=100, n_init=1,
                verbose=opts.verbose)
```

```
print("Clustering sparse data with %s" % km)
t0 = time()
km.fit(X)
print("done in %0.3fs" % (time() - t0))
print()
```

```
Clustering sparse data with KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=100,
    n_clusters=4, n_init=1, n_jobs=1, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=True)
Initialization complete
Iteration  0, inertia 6464.681
Iteration  1, inertia 3297.729
Iteration  2, inertia 3281.166
Iteration  3, inertia 3277.920
Iteration  4, inertia 3276.435
Iteration  5, inertia 3274.901
Iteration  6, inertia 3273.224
Iteration  7, inertia 3271.565
Iteration  8, inertia 3270.516
```

Plotting the Results

- Most important words in each cluster
  - Highest weights in cluster centers

```python
order_centroids = km.cluster_centers_.argsort()[:, ::-1]
for i in range(true_k):
    print("Cluster %d:" % i, end='')
    for ind in order_centroids[i, :10]:
        print(' %s' % terms[ind], end='')
    print()
```

```
Cluster 0: graphics com university image posting thanks host nntp computer ac
Cluster 1: god com people don say jesus article think bible christian
Cluster 2: space nasa henry access digex toronto pat alaska gov shuttle
Cluster 3: sandvik sgi livesey com kent apple keith newton solntze wpd
```

Confusion Matrix

- Estimated clusters vs. true categories
- Can you see where it got confused?

```
labelkm = km.labels_
from sklearn.metrics import confusion_matrix
C = confusion_matrix(labels,labelkm)

Csum = np.sum(C,axis=0)
Cnorm = C / Csum[None,:]
print(Cnorm)
```

```
[[ 0.02664797  0.5559633   0.          0.6512605 ]
 [ 0.67461431  0.00458716  0.00947867  0.        ]
 [ 0.24263675  0.01651376  0.98420221  0.        ]
 [ 0.05610098  0.42293578  0.00631912  0.3487395 ]]
```

```
dataset.target_names
```

```
['alt.atheism', 'comp.graphics', 'sci.space', 'talk.religion.misc']
```

An Example "Wrong" cluster

```
Actual newsgroup: talk.religion.misc
Most common newsgroup in cluster:  alt.atheism

From: skinner@sp94.csrd.uiuc.edu (Gregg Skinner)
Subject: Re: Davidians and compassion
Reply-To: g-skinner@uiuc.edu
Organization: UIUC Center for Supercomputing Research and Development
Lines: 26

sandvik@newton.apple.com (Kent Sandvik) writes:

>In article <1993Apr20.143400.569@ra.royalroads.ca>, mlee@post.RoyalRoads.ca
>(Malcolm Lee) wrote:
>> Do you judge all Christians by the acts of those who would call
>> themselves Christian and yet are not?  The BD's contradicted scripture
>> in their actions.  They were NOT Christian.  Simple as that.  Perhaps
>> you have read too much into what the media has portrayed.  Ask any
>> true-believing Christian and you will find that they will deny any
>> association with the BD's.  Even the 7th Day Adventists have denied any
>> further ties with this cult, which was what they were.

>Well, if they were Satanists, or followers of an obscure religion,
>then I would be sure that Christians would in unison condemn and
>make this to a show case.

You might be sure, but you would also be wrong.

>And does not this show the dangers with religion -- in order
>word a mind virus that will make mothers capable of letting
>their small children burn to ashes while they scream?

I suspect the answer to this question is the same as the answer to,
"Do not the actions of the likes of Stalin show the dangers of
atheism?"
```

- ❑ Post is from talk.religion.misc
- ❑ Placed in cluster with mostly alt.atheism

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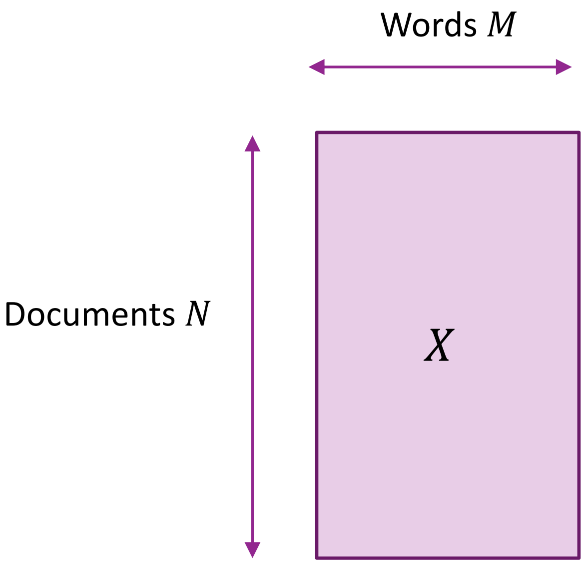
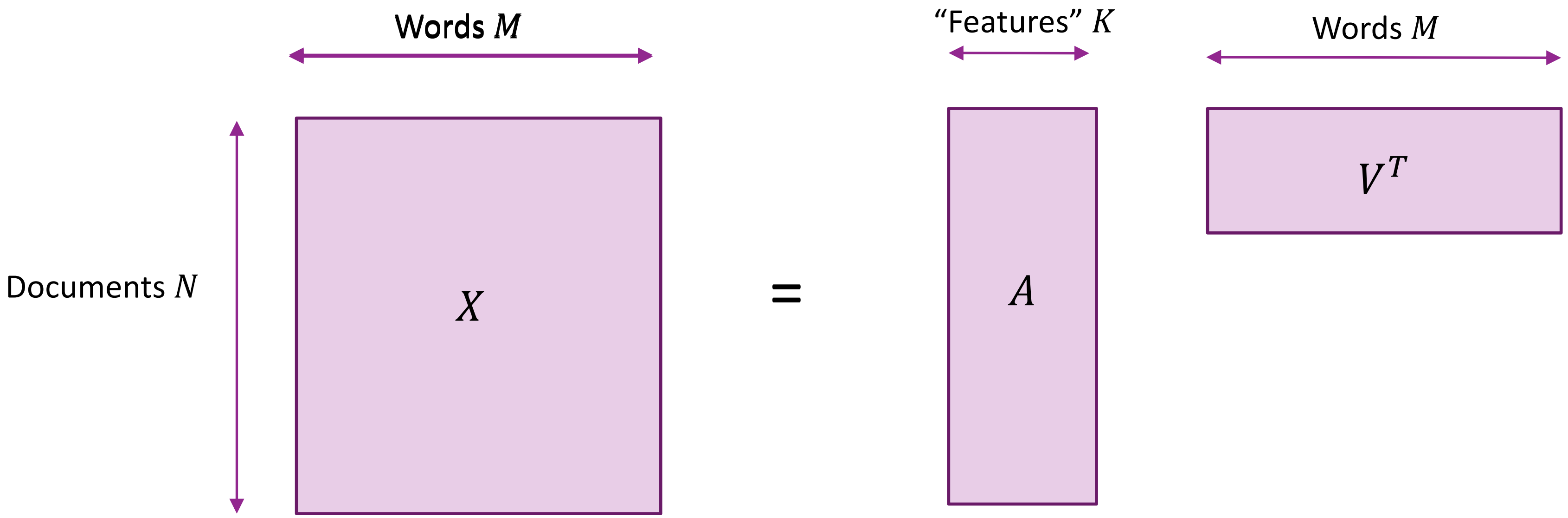
Need for Dimensionality Reduction

- Term-document matrix X is large
  - N documents $\times M$ words in vocabulary
- M is large
  - Can be 10^6 in commercial systems
- Document represented by long sparse vector
- Inefficient
- Need dimensionality reduction



Latent Semantic Analysis (PCA revisited!)

- LSA = PCA on term-document matrix
- $X \approx USV^T = AV^T, \quad A = US$
  - U, S, V^T computed by low-rank SVD



LSA Interpretation

- Each PC represents a “topic” or “concept”
- PC decomposition:

$$X[n,i] \approx \sum_{k=1}^{K} A[n,k]V[i,k]$$

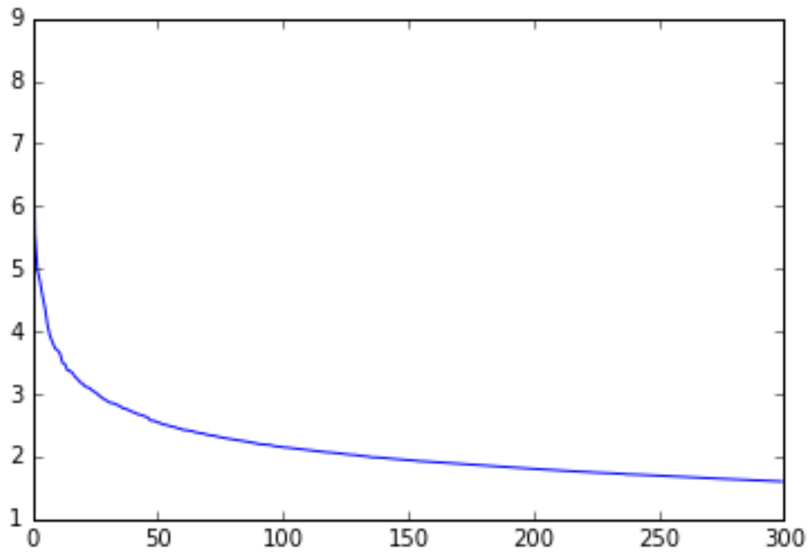
  - $A[n,k]$ = component of topic k in document n
  - $V[i,k]$ = component of word i in topic k

- Learn much more (in advanced ML class):
  - Word and document embeddings
  - Latent Dirchelet Allocation
  - ...

Perform LSA on NewsGroup

```
import scipy.sparse.linalg
U1,S1,V1 = scipy.sparse.linalg.svds(X,k=300)
```

```
plt.plot(S1[::-1])
```



- Use sparse SVD
- Much faster
- Concentration of variance in small number of PCs
- More interesting results in larger corpi

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Mixture Models

- Sometimes useful to have a probabilistic model of clustering
- Assume the underlying data samples come from K distributions (each distribution = one mixture (or component or cluster)).
- Given x, we use z(x) to represent the mixture/cluster it belongs to.
- Random variable $z \in \{1, \dots, K\}$
  - Some discrete event with PMF: $P(z = i) = q_i$
  - Typically not observed directly
  - Called a latent variable
- Observed variable x, can be continuous
  - Probability depends on z, $p(x|z = i)$
  - One PDF per mixture (or state) $z = i$
  - Each PDF is called a component

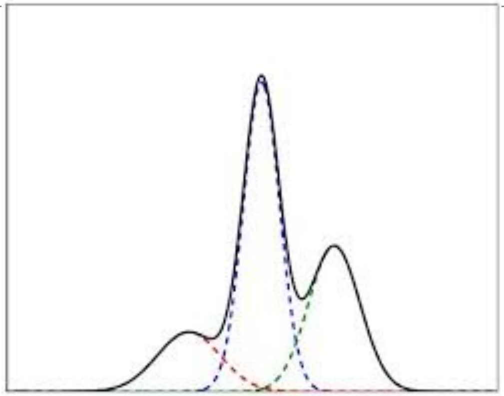
Examples

- Many data occurs from underlying discrete states
- Example 1: Size of a webpage
  - z = content of the webpage, e.g. number of images
- Example 2: Speech
  - z = phoneme the speaker is saying
- Example 3: Image
  - x = RGB values of a pixel or region of pixels
  - $z =$ one a small number of objects the pixel is part of

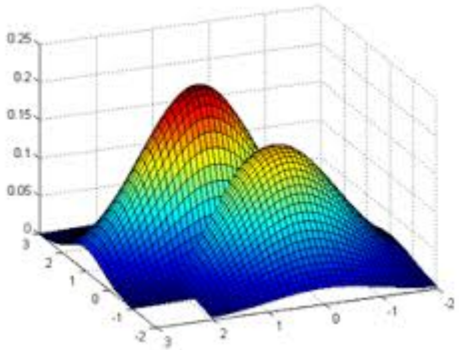
Gaussian Mixture Models

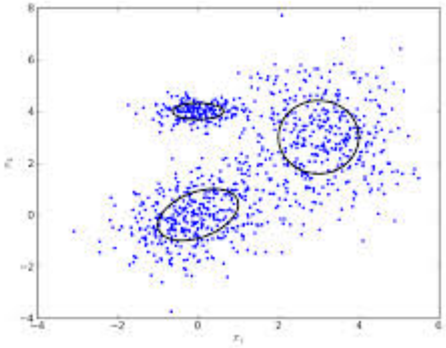
- Each $p(x|z=i)$ is a Gaussian: $N(x;\ \mu_i, P_i) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|P_i|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu_i)^T P_i^{-1}(x-\mu_i)\right\}$
- Parametrized by:
  - $q_i = P(z=i)$ = Probability of each component (Prior probability of z)
  - $\mu_i = E(x|z=i), P_i = var(x|z=i) = E\{(x-\mu_i)(x-\mu_i)^T\}$
    mean and variance in each component
- Can be vector valued
- Distribution of x can be computed via total probability
  - PDF $p(x) = \sum p(x|z=i)P(z=i) = \sum q_i N(x;\ \mu_i, P_i)$
  - CDF $F(x_0) = \sum P(x \le x_0|z=i)P(z=i)$

Visualizing GMMs



- 1d model with $K = 3$ components





- PDF for 2d GMM with $K = 2$ components
- Random points from a GMM with $K = 3$ components

Determining the Component

- Given x, can we determine z
- Use Bayes' rule:

$$P(z=i|x) = \frac{P(x|z=i)q_i}{\sum_k P(x|z=k)q_k} \quad (\text{Posterior Probability of z given x})$$

- Example: Scalar Gaussian with two components: (μ_1, σ^2) and (μ_2, σ^2), $q_1 = q_2 = 0.5$

$$P(z=1|x) = \frac{e^{-(x-\mu_1)^2/2\sigma^2}}{e^{-(x-\mu_1)^2/2\sigma^2} + e^{-(x-\mu_2)^2/2\sigma^2}} = \frac{1}{1+e^{-a(x-b)}}$$

  - Sigmoid shape
  - $a = (\mu_2 - \mu_1)/\sigma^2 =$ SNR
  - $b = (\mu_2 + \mu_1)/2 =$ center
  - Logistic regression for binary classification assumes that the discriminant function of each class follows a Gaussian distribution with the same variance!

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Maximum Likelihood Estimation

- Unknown parameters in GMM: $\theta = (q_1, \ldots, q_K, \mu_1, \ldots, \mu_K, P_1, \ldots, P_K)$
- Data $x = (x_1, \ldots, x_N)$
- Negative log likelihood:

$$L(\theta) = -\ln p(x|\theta) = -\sum_{n=1}^{N} \ln \left[\sum_{i=1}^{K} q_i N(x_n|\mu_i, P_i) \right]$$

- ML estimation:

$$\hat{\theta} = \arg\min L(\theta)$$

  - No simple way to directly optimize
  - Likelihood is non-convex

Expectation Maximization

- Negative log likelihood:

$$L(\theta) = -\ln p(x|\theta) = -\sum_{n=1}^{N} \ln\left[\sum_{i=1}^{K} q_i N(x_n|\mu_i, P_i)\right]$$

- Iterative procedure:
  - Generates a sequence of estimates $\hat{\theta}^0, \hat{\theta}^1, \ldots$

- Attempts to approach MLE

$$\hat{\theta}^k \to \arg\min_{\theta} L(\theta)$$

EM Steps

- E-step: Estimate the latent variables z (E= expectation)
  - Find the posterior of the latent variables given $\hat{\theta}^k$: $\gamma_{ni} = P\left(z = i \middle| x_n, \theta = \hat{\theta}^k\right)$
- M-step: Update parameters to minimize $L(\theta)$ (M= maximization)

$$\hat{\theta}^{k+1} = \arg\max_{\theta} Q\left(\theta, \hat{\theta}^k\right)$$

E-Step for a GMM: Finding the posterior

- Given parameters q_i, μ_i, P_i
- Find posterior by Bayes rule

$$\gamma_{ni} = P(z_n = i|x_n) = \frac{P(x_n|z_n = i)q_i}{\sum_k P(x_n|z_n = k)q_k} = \frac{N(x_n|\mu_i, P_i)q_i}{\sum_k N(x_n|\mu_k, P_k)q_k}$$

- A “soft” selection

M-Step for the GMM

- Given γ_{ni}, minimize $L(\theta)$
- Update for q_i

$$q_i = \frac{N_i}{\sum_j N_j}, \qquad N_i = \sum_n \gamma_{ni}$$

- Update for μ_i

$$\mu_i = \frac{1}{N_i} \sum_n \gamma_{ni}\, x_n$$

- Update for P_i

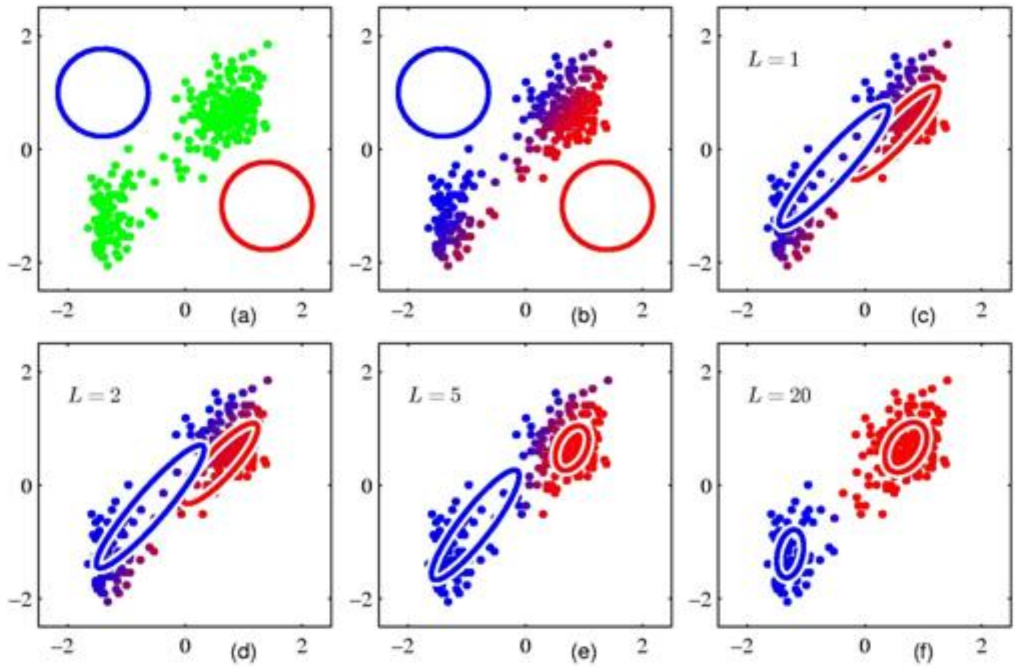
$$P_i = \frac{1}{N_i} \sum_n \gamma_{ni}\, (x_n - \mu_i)(x_n - \mu_i)^T$$

- Proof for the update for μ_i : on board
- Fore more details, See Sec. 9.2.2 in Bishop

Relation to K-Means

- EM can be seen as a "soft" version
  - In K-Means: $\gamma_{ni} = 1$ or 0
- Variance
  - In K-means: $P_i = I$ (by the use of Euclidean distance)
  - In EM, this is estimated
- EM provides "scaling" of various features by their variances and also consider the possible correlation among the feature
- EM will always converge
- EM can also be stuck to local minimum
- Important to select good initials: Initialize by K-means results!

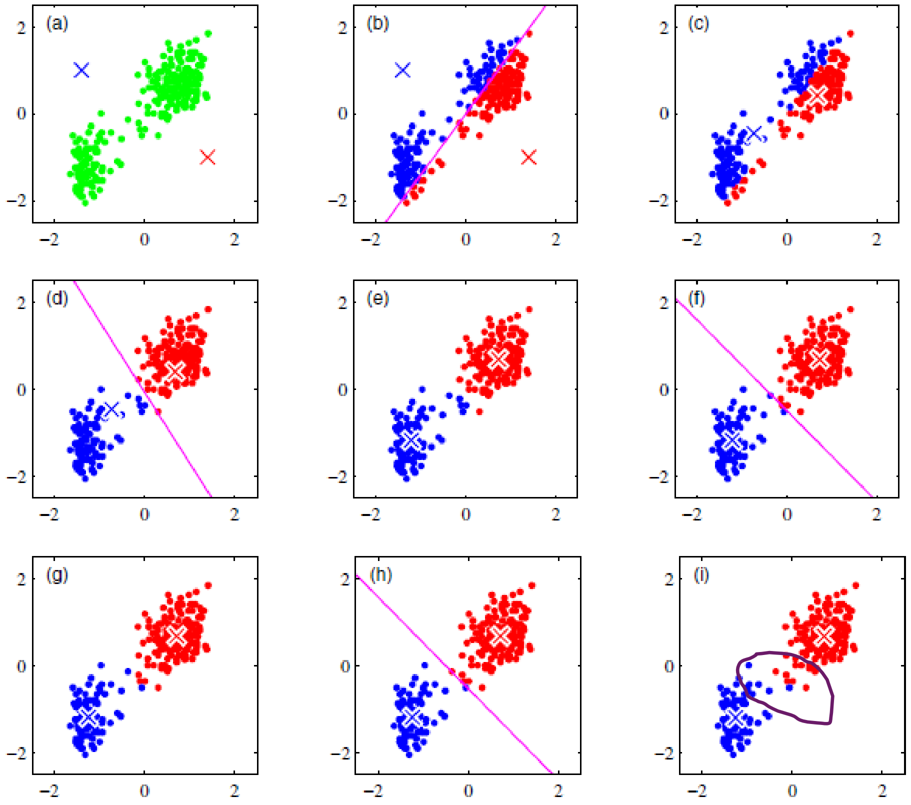
EM Illustrated



- Simple example with K=2 clusters
- Dimension = 2
- Can have bad convergence from poor initial condition

Fig. 9.8 in Bishop

K-Means illustrated



- From Bishop, Chapter 9.
- K-Means on "old faithful" data set

EM via sklearn

http://scikit-learn.org/stable/modules/generated/sklearn.mixture.GaussianMixture.html#sklearn.mixture.GaussianMixture

class sklearn.mixture.GaussianMixture(*n_components=1*, *covariance_type='full'*, *tol=0.001*, *reg_covar=1e-06*, *max_iter=100*, *n_init=1*, *init_params='kmeans'*, *weights_init=None*, *means_init=None*, *precisions_init=None*, *random_state=None*, *warm_start=False*, *verbose=0*, *verbose_interval=10*)[source]¶

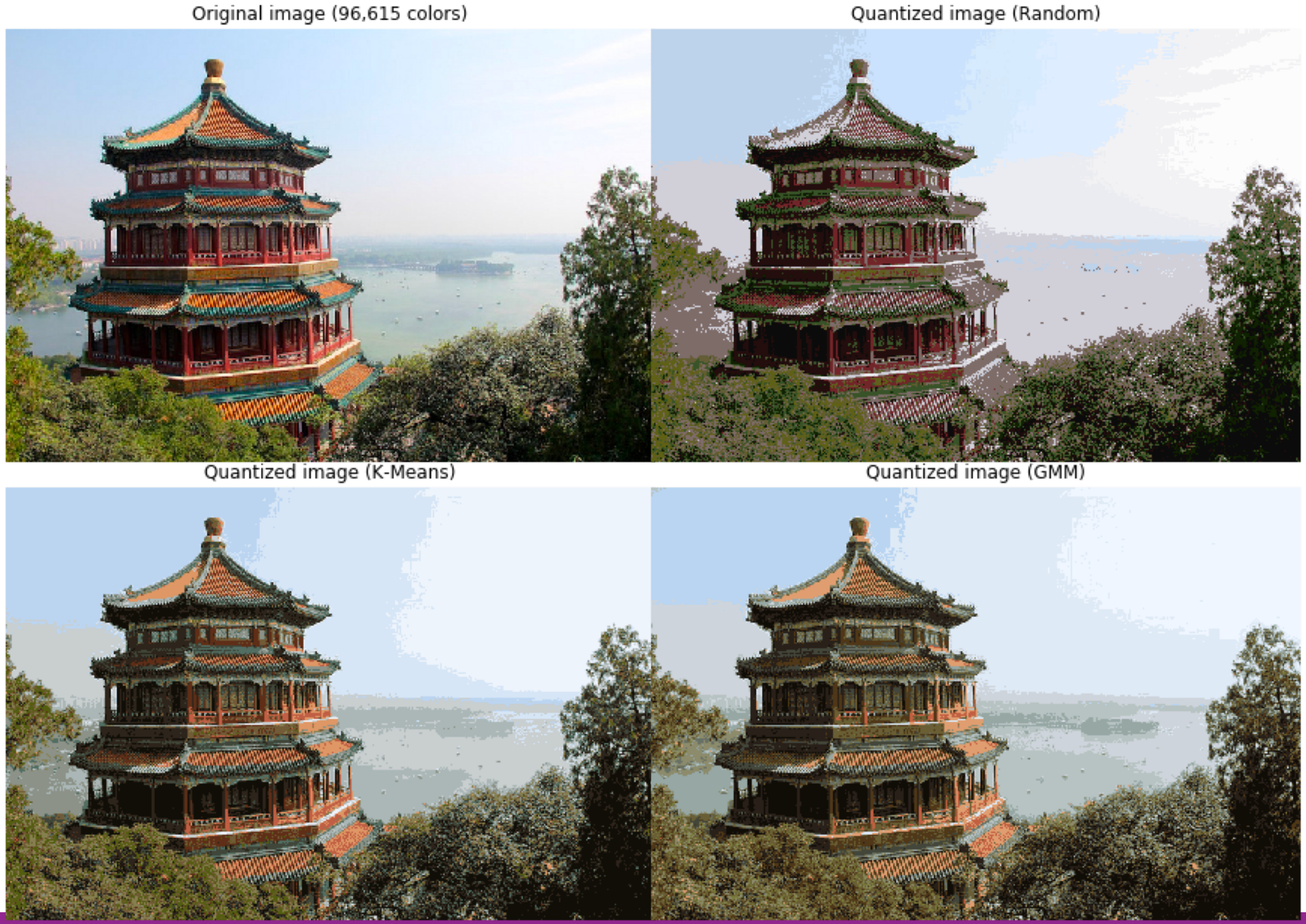
covariance_type : {'full', 'tied', 'diag', 'spherical'},

'full' (each component has its own general covariance matrix), 'tied' (all components share the same general covariance matrix), 'diag' (each component has its own diagonal covariance matrix), 'spherical' (each component has its own single variance).

- Example:

http://scikit-learn.org/stable/auto_examples/mixture/plot_gmm_covariances.html#sphx-glr-auto-examples-mixture-plot-gmm-covariances-py

Color quantization through clustering



Quantize to 16 colors only

Kmeans_GMM_color_quantization.ipynb

Other applications of clustering to images

- Image compression
  - Each image block is “quantized” to one cluster pattern, and the entire block is described by the cluster index
- Image segmentation
  - Each pixel is described by a color/texture descriptor and classified into one of the clusters
- Image classification through “Bad of Words” representation

Bag of words representation for images

- A image consists of many passible local patterns.
- How to describe the pattern of the entire image?
- Can divide an image into many small patches and cluster all patches into a few representative patterns (visual words)
- Describe an image by the frequency of each word in the image (Bag of Visual Words)
- Instead of using all patches in an image, can detect “key feature points” and quantize the descriptor for each key point into a word
- Most successful methods for image classification before deep learning

How to determine the number of clusters?

- Brute force:
  - Evaluate the cost function for different candidate numbers, on the validation set

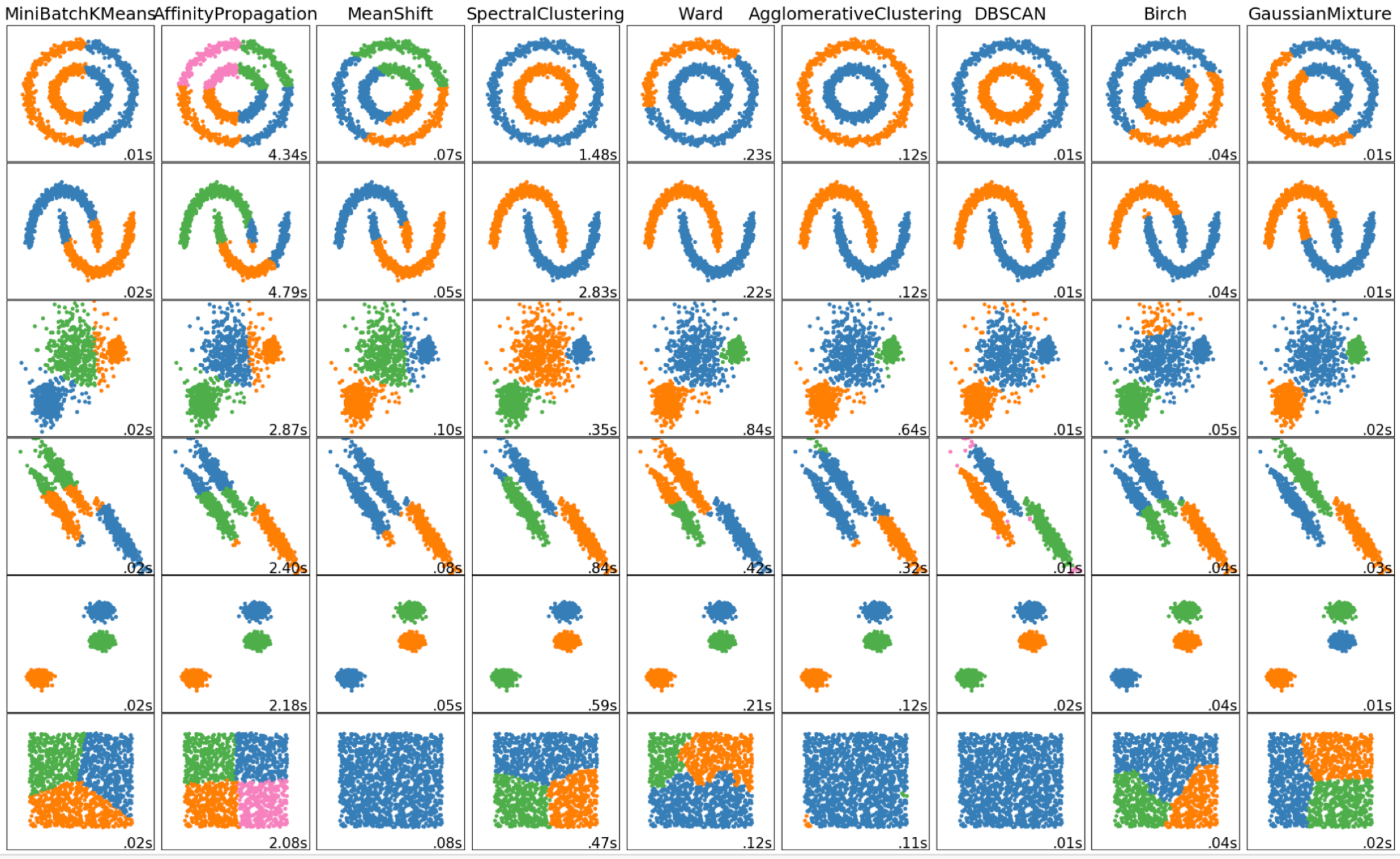
- Other methods

Other clustering methods

- K-means and EM must know the number of clusters
  - To determine the ”optimal” number: Evaluate the cost function for different candidate numbers, on the validation set
- Clustering methods that can determine the number of clusters automatically
  - Mean-shift (mode-seeking)
  - Dirichlet Process Mixture Model
  - Affinity propagation
  - …
- What features to use?
  - Application dependent
  - PCA can be used for feature dimension reduction
  - Non-linear feature learning: Spectral clustering

Examples in sklearn

- http://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py



Deep learning for clustering (unsupervised learning)

- ❑DEEP EMBEDDED CLUSTERING (DEC)
  - Using an auto encoder to learn the latent features, which are then clustered by k-means

- ❑DEEP CLUSTERING NETWORK (DCN)
  - The network is trained using sum of the signal reconstruction error and the clustering loss after k-means

- ❑CLUSTERING CNN (CCNN)

- ❑Using Generative network

From: Clustering with Deep Learning: Taxonomy and New Methods, Elie Aljalbout, Vladimir Golkov, Yawar Siddiqui, Daniel Cremers, https://arxiv.org/pdf/1801.07648.pdf

What you should know from this lecture

- What is clustering?
  - Unsupervised!
- K-means method
- GMM method
- Relationship between K-means and GMM
- Sensitivity of K-means/GMM to initial conditions