Unit 12
Clustering, K-Means, NMF, GMM, & EM

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ECE 5307: Introduction to Machine Learning, Sp23

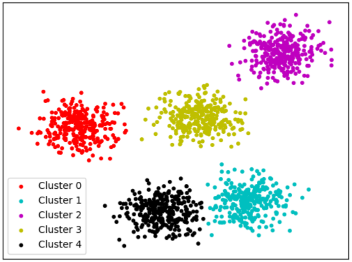
Learning objectives

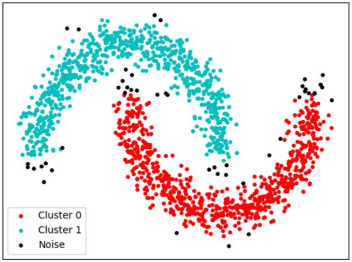
- Understand the k-means clustering objective and Lloyd's algorithm
- Understand term-document matrices and TF-IDF scores for text-mining
- Understand NMF, its relation to PCA and application to clustering
- Understand GMMs and their application to clustering
- Understand the EM algorithm and its application to GMM parameter fitting

Outline

Clustering

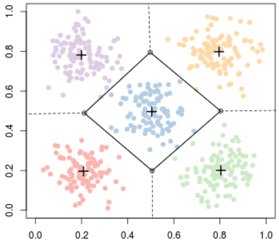
- Say we have a dataset $\{\boldsymbol{x}_i\}_{i=1}^n$ with samples $\boldsymbol{x}_i \in \mathbb{R}^d$
- Goal: Partition the dataset into K groups, where samples are similar within a group and different across groups
  - Called "clustering"
  - "Similar" may mean close in Euclidean distance, or some other metric
  - This is an unsupervised learning task; there are no labels





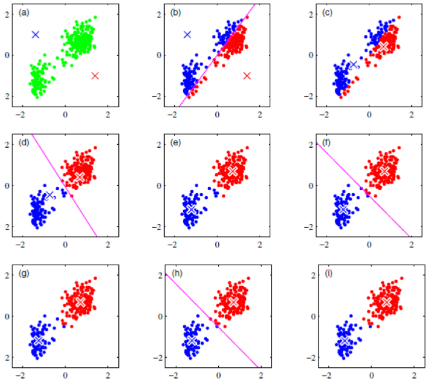
K-means clustering

- Idea: Design K centroids $\boldsymbol{C} = [\boldsymbol{c}_1, \dots, \boldsymbol{c}_K]$ that minimize the RSS cost
$$J(\boldsymbol{C}) \triangleq \sum_{i=1}^{n} \min_{k=1\dots K} \|\boldsymbol{x}_i - \boldsymbol{c}_k\|^2$$
  - This cost is the sum-squared distance from each sample to the *closest* centroid
- Define the kth cluster as the samples in $\{\boldsymbol{x}_i\}$ closest to $\boldsymbol{c}_k$
  - The cluster label given to $\boldsymbol{x}_i$ is
$$\widehat{\kappa}(\boldsymbol{x}_i) \triangleq \arg\min_{k=1\dots K} \|\boldsymbol{x}_i - \boldsymbol{c}_k\| \in \{1, \dots, K\}$$
  - The decision regions are Voronoi cells:



Lloyd's algorithm

- Lloyd's algorithm is often used to (approximately) solve the k-means problem
- The algorithm iterates two steps (given some initialization of centroids $\{\boldsymbol{c}_k\}$)
  1. For each k: compute sample mean $\boldsymbol{\mu}_k$ of data $\{\boldsymbol{x}_i\}$ within kth Voronoi cell
  2. For each k: Set new centroid at sample mean, i.e., $\boldsymbol{c}_k \leftarrow \boldsymbol{\mu}_k$
- Problem: Can get stuck in local minimum of cost
- Improvement: Careful initialization
  - k-means++ is most famous approach, but still suboptimal
  - ++ initialization used by default in sklearn.cluster.KMeans

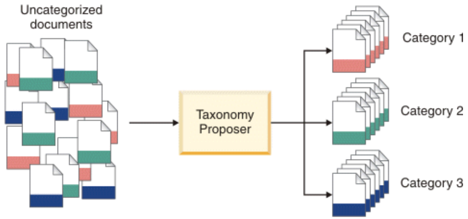


Bishop, *Pattern Recognition and Machine Learning*, 2006

Outline

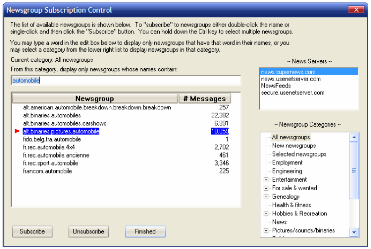
Document clustering

- Say you have a huge corpus (i.e., collection) of documents
- How do you organize them?
- Idea: Documents can be clustered
  - Grouped into similar categories
  - An example of "text mining" or "natural language processing"
- How exactly do we do this?



Example: UseNet newsgroup articles

- UseNet was an online discussion forum for various topics
  - Started on university networks in late 1970s
  - Migrated to internet, peaked in 1990s
- Useful for studying document clustering
  - UseNet documents are relatively simple and resemble emails
  - Each is labeled by the UseNet category



Newsgroup Subscription Control

The list of available newsgroups is shown below. To "subscribe" to newsgroups either double-click the name or single-click and then click the "Subscribe" button. You can hold down the Ctrl key to select multiple newsgroups.

You may type a word in the edit box below to display only newsgroups that have that word in their names, or you may select a category from the lower right list to display newsgroups in that category.

Current category: All newsgroups

From this category, display only newsgroups whose names contain:

automobile

Newsgroup	# Messages
alt.american.automobile.breakdown.breakdown.breakdown	257
alt.binaries.automobiles	22,382
alt.binaries.automobiles.carshows	6,991
alt.binaries.pictures.automobile	10,059
fido.belg.fra.automobile	1
fr.rec.automobile.4x4	2,702
fr.rec.automobile.ancienne	461
fr.rec.sport.automobile	3,346
francom.automobile	225

-- News Servers --

news.supernews.com
news.usenetserver.com
NewsFeeds
secure.usenetserver.com

-- Newsgroup Categories --

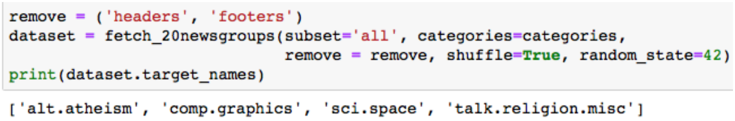
All newsgroups
New newsgroups
Selected newsgroups
Employment
Engineering
Entertainment
For sale & wanted
Genealogy
Health & fitness
Hobbies & Recreation
News
Pictures/sounds/binaries

20Newsgroups dataset

- The 20Newsgroups dataset contains . . .
  - data from 20 UseNet categories
  - $\sim$ 1000 documents/category

comp.graphics comp.os.ms-windows.misc comp.sys.ibm.pc.hardware comp.sys.mac.hardware comp.windows.x	rec.autos rec.motorcycles rec.sport.baseball rec.sport.hockey	sci.crypt sci.electronics sci.med sci.space
misc.forsale	talk.politics.misc talk.politics.guns talk.politics.mideast	talk.religion.misc alt.atheism soc.religion.christian

- The 20Newsgroups dataset is available via sklearn
  - We will load only 4 categories, resulting in 3387 total samples

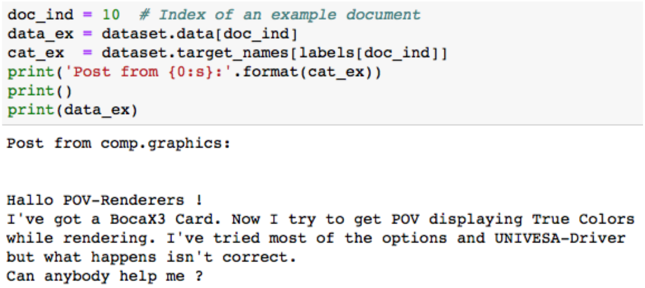


```
remove = ('headers', 'footers')
dataset = fetch_20newsgroups(subset='all', categories=categories,
                             remove = remove, shuffle=True, random_state=42)
print(dataset.target_names)
```

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

20Newsgroups dataset (cont.)

- Data is loaded into ...
  - `dataset.data`: an array of UseNet posts (represented as strings)
  - `dataset.labels`: an array of class labels (i.e., post categories)
  - `dataset.target_names`: the title of each category
- An example UseNet post:



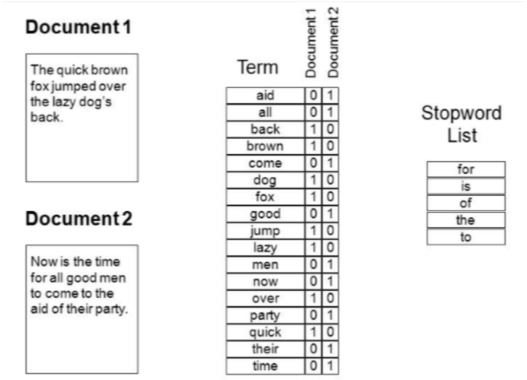
```
doc_ind = 10  # Index of an example document
data_ex = dataset.data[doc_ind]
cat_ex  = dataset.target_names[labels[doc_ind]]
print('Post from {0:s}:'.format(cat_ex))
print()
print(data_ex)
```

```
Post from comp.graphics:


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 ?
```

Outline

Bag-of-words model

- To apply k-means to document classification, we must somehow extract *numerical features* from our documents
- A simple approach is the bag-of-words model:
  - List all words (or "terms")
  - Represent each document by its vector of word counts
  - But omit common words, like "the" (called "stopwords")
- Challenges:
  - Some documents are much longer than others
  - Some terms are much more common than others



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

TF-IDF features

- So instead use ...
  - $\mathrm{TF}[i,j] = \dfrac{\text{\# occurrences of term } j \text{ in doc } i}{\text{\# terms in doc } i}$, "term frequency"
    - invariant to document size
  - $\mathrm{IDF}[j] = -\log\left(\dfrac{\text{\# docs with term } j \text{ in corpus}}{\text{\# docs in corpus}}\right)$, "inverse document frequency"
    - emphasizes uncommon terms
- The TF-IDF features $\boldsymbol{X} = [\boldsymbol{x}_1, \dots, \boldsymbol{x}_n]^\mathsf{T}$ are usually constructed as

$$X[i,j] = \mathrm{TF}[i,j]\,\mathrm{IDF}[j]$$

  - Used by 83% of text recommender systems as of 2015!
  - Note: in much of the literature, $\boldsymbol{X}$ above is transposed
    - We write it as above to be consistent with our earlier lectures
- $\boldsymbol{X}^\mathsf{T}$ is often called the "term-document" matrix

The term-document matrix

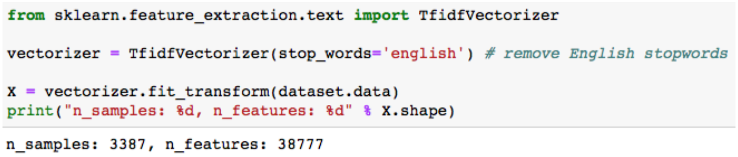
- The term-document matrix $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ has many uses
  - Recall $X[i,j]$ is the TF-IDF score of document i and term j
- In document retrieval, the goal is to find which documents are most associated with a given term or terms
  - Used for search engines (e.g., Google, Microsoft Bing)
  - Simple approach: Given term j, extract jth column of $\boldsymbol{X}$, i.e., $\boldsymbol{d}_j \triangleq [\boldsymbol{X}]_{:,j}$
  - The most relevant documents have the highest scores in the "document vector" $\boldsymbol{d}_j$
- In semantic analysis, one wants to find relationships among terms
  - Used to extract language-independent meaning from text
  - Simple approach: Given terms (j, j'), compute $\boldsymbol{d}_j^{\mathsf{T}} \boldsymbol{d}_{j'}$ to measure their similarity

Term-document structure

- Challenge: The term-document matrix $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ can be huge!
  - $n = \#$ documents in corpus
  - $d = \#$ terms in vocabulary (38777 even in our small demo!)
- Fortunately, $\boldsymbol{X}$ tends to be sparse
  - Sparse means most elements are zero-valued
  - Sparsity implies that most documents use only a small fraction of the vocabulary
  - Representing $\boldsymbol{X}$ as a sparse matrix can help to reduce its memory footprint
- And often $\boldsymbol{X}$ has low rank (i.e., few non-zero eigenvalues)
  - We can exploit this for document clustering!
- Finally, note that $X[i,j] \geq 0$ for all i and j
  - We can also exploit this for document clustering!

Computing TF-IDF in Python

- To compute TF-IDF features $\boldsymbol{X}$, we can use sklearn's TfidfVectorizer method:



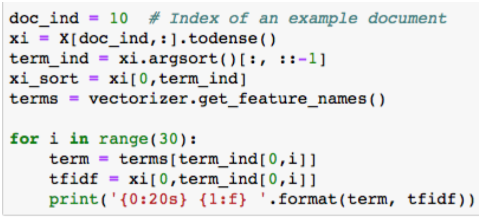
```
from sklearn.feature_extraction.text import TfidfVectorizer

vectorizer = TfidfVectorizer(stop_words='english') # remove English stopwords

X = vectorizer.fit_transform(dataset.data)
print("n_samples: %d, n_features: %d" % X.shape)
```

```
n_samples: 3387, n_features: 38777
```

- We can then run k-means on the term-document matrix $\boldsymbol{X}$ in an attempt to cluster documents

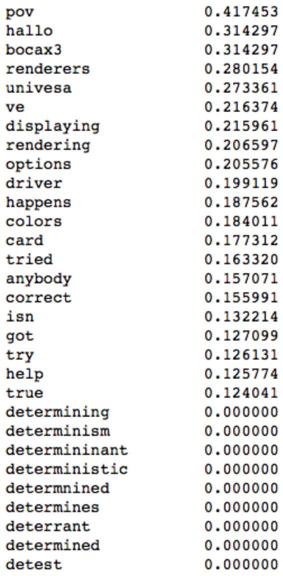
Example TF-IDF scores

- For an example document, the terms with the highest TF-IDF scores are shown on the right:



```python
doc_ind = 10  # Index of an example document
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))
```

- Note that this is the same `comp.graphics` post that we saw earlier, on page 11



```
pov                  0.417453
hallo                0.314297
bocax3               0.314297
renderers            0.280154
univesa              0.273361
ve                   0.216374
displaying           0.215961
rendering            0.206597
options              0.205576
driver               0.199119
happens              0.187562
colors               0.184011
card                 0.177312
tried                0.163320
anybody              0.157071
correct              0.155991
isn                  0.132214
got                  0.127099
try                  0.126131
help                 0.125774
true                 0.124041
determining          0.000000
determinism          0.000000
determininant        0.000000
deterministic        0.000000
determnined          0.000000
determines           0.000000
deterrant            0.000000
determined           0.000000
detest               0.000000
```

Running k-means

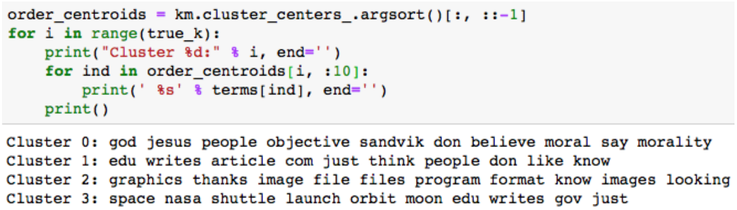
- We can use sklearn.cluster.KMeans to implement k-means:

```
np.random.seed(1) # to make repeatable

from sklearn.cluster import KMeans, MiniBatchKMeans
km = KMeans(n_clusters=true_k, init='k-means++', max_iter=100, n_init=1,
                verbose=True)
km.fit(X)
```

```
Initialization complete
Iteration  0, inertia 6387.081
Iteration  1, inertia 3298.568
Iteration  2, inertia 3286.525
Iteration  3, inertia 3281.397
Iteration  4, inertia 3277.493
Iteration  5, inertia 3276.394
Iteration  6, inertia 3276.072
Iteration  7, inertia 3275.957
Iteration  8, inertia 3275.905
Iteration  9, inertia 3275.871
Iteration 10, inertia 3275.855
Iteration 11, inertia 3275.843
Iteration 12, inertia 3275.833
Iteration 13, inertia 3275.831
Converged at iteration 13: center shift 0.000000e+00 within tolerance 9.816505e-09

KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=100,
    n_clusters=4, n_init=1, n_jobs=None, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=True)
```

Result of k-means clustering

- Recall that, in this example, we asked k-means to compute $K = 4$ centroids:
  - Each centroid is a 38777-length vector of TF-IDF scores
  - Each score corresponds to a particular term
- Let's print the terms with the 10 top TF-IDF scores in each centroid:



```
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: god jesus people objective sandvik don believe moral say morality
Cluster 1: edu writes article com just think people don like know
Cluster 2: graphics thanks image file files program format know images looking
Cluster 3: space nasa shuttle launch orbit moon edu writes gov just
```

  - We can see some correspondence with the true categories:

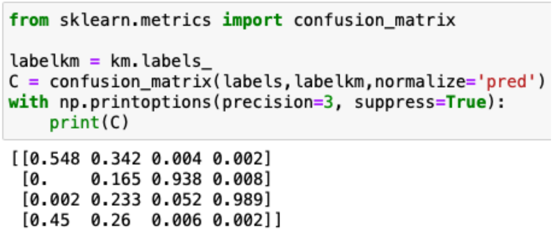
```
['alt.atheism', 'comp.graphics', 'sci.space', 'talk.religion.misc']
```

  - But the categorization is not perfect

Confusion matrix

- To better understand the relationship between the k-means clusters and the true categories, we can compute a (normalized) confusion matrix $\boldsymbol{C}$:

$$C[l,k] \triangleq \text{the fractional contribution of true-category } l \text{ to cluster } k$$



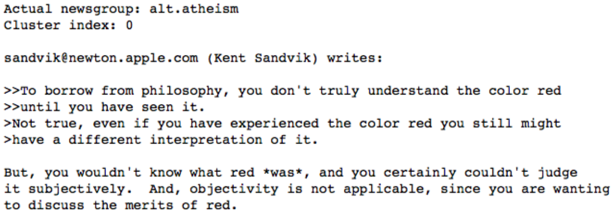
```python
from sklearn.metrics import confusion_matrix

labelkm = km.labels_
C = confusion_matrix(labels,labelkm,normalize='pred')
with np.printoptions(precision=3, suppress=True):
    print(C)
```

```
[[0.548 0.342 0.004 0.002]
 [0.    0.165 0.938 0.008]
 [0.002 0.233 0.052 0.989]
 [0.45  0.26  0.006 0.002]]
```

- Looking at the columns of the confusion matrix, we see that . . .
  - cluster $k = 0$ is split between `alt.atheism` and `talk.religion.misc`
  - cluster $k = 1$ is a mix of all four newsgroups
  - cluster $k = 2$ is dominated by posts from `comp.graphics`
  - cluster $k = 3$ is dominated by posts from `sci.space`

An example clustering “error”

- Recall that cluster $k = 2$ was dominated by `comp.graphics`
- But a small number of `alt.atheism` posts were included
- One such post is on the right
- Not surprising that this post was clustered with `comp.graphics`, since it repeatedly uses “color” and “red”

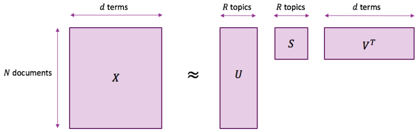


```
Actual newsgroup: alt.atheism
Cluster index: 0

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

>>To borrow from philosophy, you don't truly understand the color red
>>until you have seen it.
>Not true, even if you have experienced the color red you still might
>have a different interpretation of it.

But, you wouldn't know what red *was*, and you certainly couldn't judge
it subjectively.  And, objectivity is not applicable, since you are wanting
to discuss the merits of red.
```

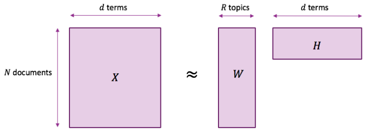
Outline

Topic modeling via low-rank matrix factorization

- By factorizing the $n \times d$ term-document matrix $\boldsymbol{X}$ into a product of $n \times R$ and $R \times d$ matrices with $R \ll r = \operatorname{rank}(\boldsymbol{X})$, we implicitly build an R-topic model.
- There are two common ways to do this:
  1. PCA: $\boldsymbol{X} \approx \boldsymbol{U}_R(\boldsymbol{S}_R\boldsymbol{V}_R^\mathsf{T})$ with $\boldsymbol{U}_R \in \mathbb{R}^{n\times R}$ and $(\boldsymbol{S}_R\boldsymbol{V}_R^\mathsf{T}) \in \mathbb{R}^{R\times d}$



  2. NMF: $\boldsymbol{X} \approx \boldsymbol{W}_R\boldsymbol{H}_R$ with $\boldsymbol{W}_R \in \mathbb{R}_+^{n\times R}$ and $\boldsymbol{H}_R \in \mathbb{R}_+^{R\times d}$



- PCA minimizes the RSS $\|\boldsymbol{X} - \widehat{\boldsymbol{X}}_R\|_F^2$.
- NMF minimizes RSS under the constraint of non-negative $\boldsymbol{W}_R$ and $\boldsymbol{H}_R$

Latent semantic analysis (PCA revisited!)

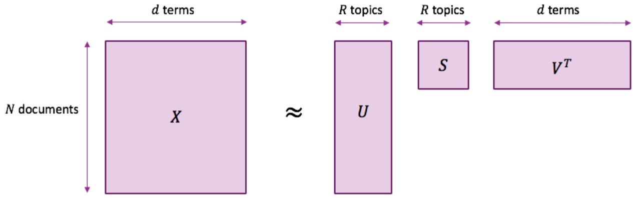
- Recall that the economy SVD decomposes $\boldsymbol{X}$ as follows:

$$\boldsymbol{X} = \boldsymbol{U}_r \boldsymbol{S}_r \boldsymbol{V}_r^{\mathsf{T}} = \sum_{k=1}^{r} \boldsymbol{u}_k s_k \boldsymbol{v}_k^{\mathsf{T}} \quad \text{where} \quad r = \operatorname{rank}(\boldsymbol{X}) \leq \min\{n, d\}$$

- And recall that PCA gives a low-rank approximation of $\boldsymbol{X}$, i.e.,

$$\boldsymbol{X} \approx \boldsymbol{U}_R \boldsymbol{S}_R \boldsymbol{V}_R^{\mathsf{T}} = \sum_{k=1}^{R} \boldsymbol{u}_k s_k \boldsymbol{v}_k^{\mathsf{T}} \quad \text{for some} \quad R \ll r$$

  - Called latent semantic analysis (LSA) when $\boldsymbol{X}$ is a term-document matrix
  - R acts as the number of "topics"



Latent semantic analysis as topic modeling

- Performing LSA on the term-document matrix $\boldsymbol{X}$ gives

$$\boldsymbol{X} \approx \boldsymbol{U}_R \boldsymbol{S}_R \boldsymbol{V}_R^{\mathsf{T}} = \sum_{k=1}^{R} \boldsymbol{u}_k s_k \boldsymbol{v}_k^{\mathsf{T}} \quad \text{for some} \quad R \ll \min\{n, d\}$$

  - $\{\boldsymbol{u}_k\}_{k=1}^R$ are the R principal document vectors in the corpus
  - $\{\boldsymbol{v}_k\}_{k=1}^R$ are the R principal term vectors in the corpus
  - $\{s_k\}_{k=1}^R$ are the R weights of the topics in the corpus
- Interpretation:
  - The corpus $\boldsymbol{X}$ can be approximated using R topics
  - $[\boldsymbol{U}_R]_{i,:}$ shows the relative contributions of document i to the R topics
  - $[\boldsymbol{V}_R]_{j,:}$ shows the relative contributions of term j to the R topics
- Challenge:
  - The values in $\boldsymbol{U}_R$ and $\boldsymbol{V}_R$ can be negative
  - How do we interpret these negative values?

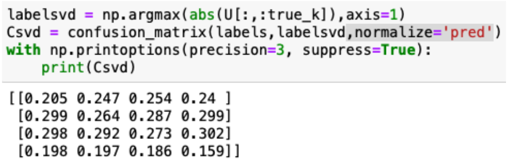
LSA/PCA on 20Newsgroups

- Let's apply LSA to cluster the 20Newsgroups data:

```
PC 0: 3do rh craig post site number vesa terrorist days society
PC 1: allah send anti test ye 3do faq actually dos posted
PC 2: phigs program new psilink p00261 zip universe thing lot send
PC 3: free polygon rle rh phigs read set siggraph convert different
```

  - For each topic k, the terms $\{j\}$ yielding the 10 largest v_{jk} components do *not* look well clustered

- If we cluster documents via $\widehat{k}(\boldsymbol{x}_i) = \arg\max_{k=1,\dots,R} u_{ik}$, the confusion matrix does *not* look good



```
labelsvd = np.argmax(abs(U[:,:true_k]),axis=1)
Csvd = confusion_matrix(labels,labelsvd,normalize='pred')
with np.printoptions(precision=3, suppress=True):
    print(Csvd)
```

```
[[0.205 0.247 0.254 0.24 ]
 [0.299 0.264 0.287 0.299]
 [0.298 0.292 0.273 0.302]
 [0.198 0.197 0.186 0.159]]
```

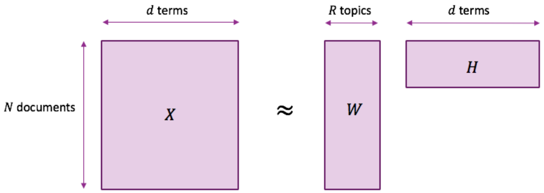
- LSA/PCA does not work well for clustering this dataset!

Nonnegative matrix factorization

- An alternative low-rank approx is nonnegative matrix factorization (NMF):

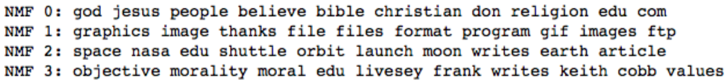
$$\boldsymbol{X} \approx \boldsymbol{W}_R \boldsymbol{H}_R \quad \text{for} \quad (\boldsymbol{W}_R, \boldsymbol{H}_R) = \underset{\boldsymbol{W}\in\mathbb{R}_+^{n\times R},\, \boldsymbol{H}\in\mathbb{R}_+^{R\times d}}{\arg\min} \|\boldsymbol{X} - \boldsymbol{W}\boldsymbol{H}\|_F^2$$

- For a given number of topics R ...
  - the approximation error is larger than with SVD, but
  - the coefs in $\boldsymbol{W}_R$ and $\boldsymbol{H}_R$ are *interpretable*: larger means more relevant



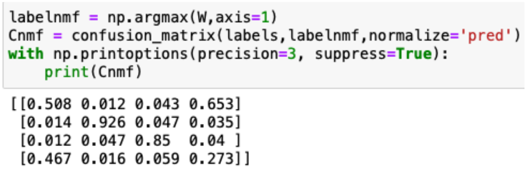
NMF on 20Newsgroups

- For each topic k, the terms $\{j\}$ yielding the 10 largest h_{kj} coefficients look well clustered!



```
NMF 0: god jesus people believe bible christian don religion edu com
NMF 1: graphics image thanks file files format program gif images ftp
NMF 2: space nasa edu shuttle orbit launch moon writes earth article
NMF 3: objective morality moral edu livesey frank writes keith cobb values
```

- If we cluster documents via $\widehat{\kappa}(\boldsymbol{x}_i) = \arg\max_{k=1,\dots,R} w_{ik}$, confusion matrix looks good!
  - cluster $k=1$ dominated by `comp.graphics`
  - cluster $k=2$ dominated by `sci.space`
  - cluster $k=0,3$ mix `alt.altheism` and `talk.religion.misc`



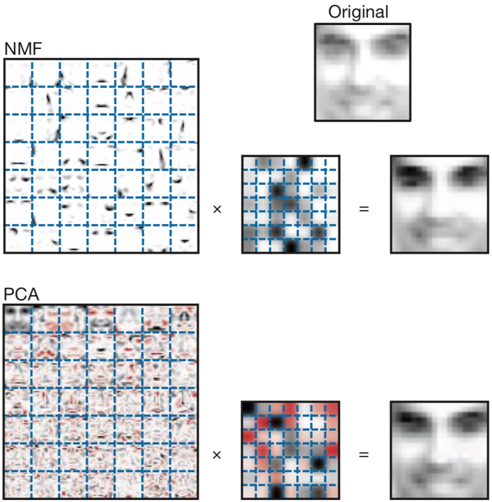
```
labelnmf = np.argmax(W,axis=1)
Cnmf = confusion_matrix(labels,labelnmf,normalize='pred')
with np.printoptions(precision=3, suppress=True):
    print(Cnmf)
```

```
[[0.508 0.012 0.043 0.653]
 [0.014 0.926 0.047 0.035]
 [0.012 0.047 0.85  0.04 ]
 [0.467 0.016 0.059 0.273]]
```

- Original categories: `['alt.atheism', 'comp.graphics', 'sci.space', 'talk.religion.misc']`

NMF versus LSA/PCA

- NMF approximates $\boldsymbol{X}$ by a *non-negative* sum of *non-negative* components
  - Yields a "parts based" representation
  - A 49-term approximation of a 1024-pixel image is shown on right
- LSA/PCA approximates $\boldsymbol{X}$ by a sum of *orthonormal* components
  - Allows subtractive combinations
  - Negative values shown as red, positive as black



Lee and Seung, "Learning the parts of objects by non-negative matrix factorization," *Nature*, 1999

NMF versus LSA/PCA

$$\boldsymbol{X} \overset{\text{NMF}}{\approx} \boldsymbol{W}_R \boldsymbol{H}_R \qquad \text{versus} \qquad \boldsymbol{X} \overset{\text{PCA}}{\approx} \boldsymbol{U}_R \boldsymbol{S}_R \boldsymbol{V}_R^{\mathsf{T}}$$

- Both are low-rank approximations
- NMF designed for non-negative $\boldsymbol{X}$ while PCA allows any $\boldsymbol{X}$
- NMF gives non-negative $\boldsymbol{W}_R, \boldsymbol{H}_R$ while PCA can have negative $\boldsymbol{U}_R, \boldsymbol{V}_R$
- NMF gives non-orthogonal $\boldsymbol{W}_R, \boldsymbol{H}_R$ while PCA gives orthogonal $\boldsymbol{U}_R, \boldsymbol{V}_R$
- NMF encourages sparse $\boldsymbol{W}_R, \boldsymbol{H}_R$ while PCA gives dense $\boldsymbol{U}_R, \boldsymbol{V}_R$
- NMF is non-unique while PCA is unique
- NMF solvers can get stuck in local minima, while PCA solvers don't

See `http://www.cs.rochester.edu/~jliu/CSC-576/NMF-tutorial.pdf`

NMF for matrix completion

- There are other important applications of NMF
- For example, recommender systems aim to recommend products to users
- Collaborative filtering is a popular approach to recommender systems:
  - Suppose that $[\boldsymbol{X}]_{ij}$ stores the rating for product i from user j
  - Challenge: Only a few entries of $\boldsymbol{X} \in \mathbb{R}_+^{n \times d}$ are known; the rest are missing
  - Goal: Fill in the missing entries in $\boldsymbol{X}$ (i.e., "matrix completion")
- To apply NMF, we model $\boldsymbol{X} \approx \boldsymbol{W}_R \boldsymbol{H}_R$ for some R and solve for

$$(\boldsymbol{W}_R, \boldsymbol{H}_R) = \underset{\boldsymbol{W} \in \mathbb{R}_+^{n \times R},\, \boldsymbol{H} \in \mathbb{R}_+^{R \times d}}{\arg\min} \sum_{i,j \text{ known}} \left([\boldsymbol{X}]_{i,j} - [\boldsymbol{W}\boldsymbol{H}]_{i,j} \right)^2$$

- A famous example is the Netflix contest, where Netflix gave \$1M to the winner
  - 18k movies, 480k users, 100M ratings (1.2% complete)

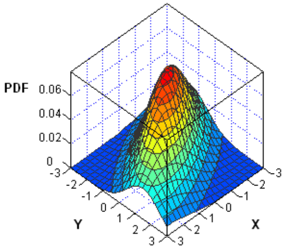
Outline

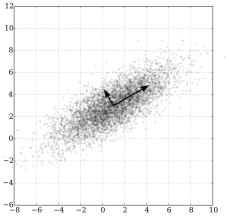
Multivariate Gaussian distribution

- Consider a multivariate Gaussian random vector $\boldsymbol{x}$
- If $\boldsymbol{x}$ has mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{Q}$, then its pdf takes the form

$$p(\boldsymbol{x}) = \underbrace{|2\pi\boldsymbol{Q}|^{-1/2}}_{\text{scale factor}} \underbrace{e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{Q}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}}_{\text{exponentiated quadratic form}} \triangleq \mathcal{N}(\boldsymbol{x};\boldsymbol{\mu},\boldsymbol{Q})$$

- The eigendecomp $\boldsymbol{Q} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{\mathsf{T}}$ determines the shape of the pdf & scatterplot
  - Contours are ellipsoidal, with principle axis $\boldsymbol{v}_k$ stretched by $\sqrt{\lambda_k}$ for $k = 1 \dots K$





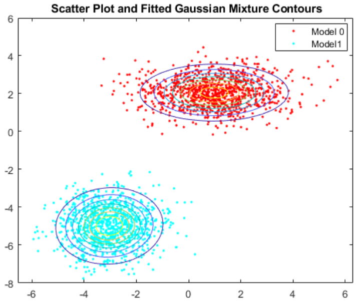
Gaussian mixture models

- A Gaussian mixture model (GMM) is a weighted sum of K Gaussian pdfs:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \gamma_k \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{Q}_k) \quad \text{with} \quad \gamma_k \geq 0 \quad \text{and} \quad \sum_{k=1}^{K} \gamma_k = 1$$

  - The kth pdf has mean $\boldsymbol{\mu}_k$ and covariance $\boldsymbol{Q}_k$
  - The weight γ_k controls the probability of the kth component

- A GMM can be used to cluster!
  - First, fit the GMM parameters $\{\boldsymbol{\mu}_k, \boldsymbol{Q}_k, \gamma_k\}$ to the dataset $\{\boldsymbol{x}_i\}_{i=1}^n$
  - Then cluster a test $\boldsymbol{x}$ by determining which GMM component k is more probable
  - This latter step is better understood by writing the GMM in a hierarchical form . . .



A hierarchical view of the GMM

- Consider a two-stage approach to generating a random vector $\boldsymbol{x}$:
  1. draw component index $\kappa \in \{1, \dots, K\}$ according to pmf $[\gamma_1, \dots, \gamma_K]$
     - Thus $\Pr\{\kappa = k\} = \gamma_k$ for $k = 1, \dots, K$
  2. then draw $\boldsymbol{x}$ according to pdf $\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_\kappa, \boldsymbol{Q}_\kappa)$, which uses that fixed value of κ
     - Thus $p(\boldsymbol{x} \,|\, \kappa = k) = \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{Q}_k)$ for $k = 1, \dots, K$

- This can be understood/justified as follows. From the law of total probability,

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} p(\boldsymbol{x}, \kappa = k) = \sum_{k=1}^{K} p(\boldsymbol{x} \,|\, \kappa = k) \Pr\{\kappa = k\} = \sum_{k=1}^{K} \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{Q}_k)\gamma_k$$

  - This matches our GMM!
  - So, can think of GMM as a two-level hierarchy: first draw κ, then draw $\boldsymbol{x}|\kappa$
  - Because κ doesn't explicitly appear in $p(\boldsymbol{x})$, it's called a "hidden variable"
    - Note: there are many other ways to identify hidden variables in $p(\boldsymbol{x})$, but this one is most convenient for our current task

Inferring the hidden variable

- Recall the hierarchical form of the GMM:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \underbrace{\Pr\{\kappa=k\}}_{\gamma_k} \, \underbrace{p(\boldsymbol{x}\,|\,\kappa=k)}_{\mathcal{N}(\boldsymbol{x};\boldsymbol{\mu}_k,\boldsymbol{Q}_k)}$$

- We will cluster the sample $\boldsymbol{x}$ by MAP estimation, i.e., we will find the most probable component index κ associated with $\boldsymbol{x}$:
  - Given $\boldsymbol{x}$, the probability that it was generated from the component k is

$$\begin{aligned}\Pr\{\kappa=k\,|\,\boldsymbol{x}\} &= \frac{p(\boldsymbol{x}\,|\,\kappa=k)\Pr\{\kappa=k\}}{p(\boldsymbol{x})} \quad \text{via Bayes rule}\\ &= \frac{\gamma_k\mathcal{N}(\boldsymbol{x};\boldsymbol{\mu}_k,\boldsymbol{Q}_k)}{\sum_{k'}\gamma_{k'}\mathcal{N}(\boldsymbol{x};\boldsymbol{\mu}_{k'},\boldsymbol{Q}_{k'})} \quad \text{called a "soft" assignment}\end{aligned}$$

  - The MAP estimate of κ would then be:

$$\widehat{\kappa}(\boldsymbol{x}) = \arg\max_{k=1\ldots K} \Pr\{\kappa=k\,|\,\boldsymbol{x}\} \quad \text{called a "hard" assignment}$$

Summary of GMM-based clustering

- GMM-based clustering of $\{\boldsymbol{x}_i\}_{i=1}^n$ is done in two steps:
  - Fit the GMM parameters $\boldsymbol{\theta} \triangleq \{\gamma_k, \boldsymbol{\mu}_k, \boldsymbol{Q}_k\}_{k=1}^K$ to the data $\{\boldsymbol{x}_i\}_{i=1}^n$
  - For each i & k, compute soft $\Pr\{\kappa_i = k \,|\, \boldsymbol{x}_i\} = \dfrac{\gamma_k \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k, \boldsymbol{Q}_k)}{\sum_{k'} \gamma_{k'} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{k'}, \boldsymbol{Q}_{k'})}$
  - For each i, compute hard assignment $\widehat{\kappa}(\boldsymbol{x}_i) = \arg\max_{k=1\dots K} \Pr\{\kappa_i = k \,|\, \boldsymbol{x}_i\}$

- To fit the GMM parameters, we'd like to use maximum-likelihood (ML):

$$\widehat{\boldsymbol{\theta}}_{\mathsf{ml}} = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{X} \,|\, \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \left\{ \ln p(\boldsymbol{X} \,|\, \boldsymbol{\theta}) \right\}$$

$$\ln p(\boldsymbol{X} \,|\, \boldsymbol{\theta}) = \sum_{i=1}^{n} \ln \left(\sum_{k=1}^{K} \gamma_k \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k, \boldsymbol{Q}_k) \right) \quad \text{assuming i.i.d. } \{\boldsymbol{x}_i\}$$

  - But this is non-convex and difficult to maximize!
  - Instead, we'll compute an approximation to $\widehat{\boldsymbol{\theta}}_{\mathsf{ml}}$ using the EM algorithm ...

Outline

Expectation maximization (EM)

- The EM algorithm is an iterative approximation to (generic) ML estimation:
  - guaranteed to converge to a local maximum of the likelihood function
  - but need a good initialization to avoid bad local maxima (if they exist)
- Main idea: Using some hidden variables $\boldsymbol{Z}$, we alternate between estimating $\boldsymbol{Z}$ and maximizing $\boldsymbol{\theta}$:

$$\begin{aligned} \mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)}) &= \mathbb{E}_{\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta}^{(t)}}\big\{\ln p(\boldsymbol{X},\boldsymbol{Z};\boldsymbol{\theta})\big\} && \text{"E step"} \\ \boldsymbol{\theta}^{(t+1)} &= \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)}) && \text{"M step"} \end{aligned}$$

- We say "estimate $\boldsymbol{Z}$" because the E step involves the belief $p(\boldsymbol{Z}\,|\,\boldsymbol{X};\boldsymbol{\theta}^{(t)})$:

$$\mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)}) = \int p(\boldsymbol{Z}\,|\,\boldsymbol{X};\boldsymbol{\theta}^{(t)}) \ln p(\boldsymbol{X},\boldsymbol{Z};\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{Z}$$

  - Note: if $p(\boldsymbol{Z}\,\big|\,\boldsymbol{X};\boldsymbol{\theta}^{(t)}) = \delta(\boldsymbol{Z}-\widehat{\boldsymbol{Z}}^{(t)})$, then $\mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)}) = \ln p(\boldsymbol{X},\widehat{\boldsymbol{Z}}^{(t)};\boldsymbol{\theta})$
  - More generally, $\mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)})$ averages $\ln p(\boldsymbol{X},\boldsymbol{Z};\boldsymbol{\theta})$ over all *probable* values of $\boldsymbol{Z}$

EM explained: Iterative maximization of lower bound

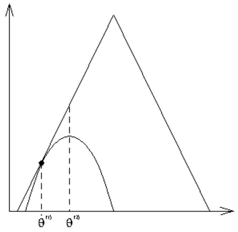
- Notice that, for any pdf $\widehat{p}(\boldsymbol{Z})$, which acts as our belief on $\boldsymbol{Z}$, we can write

$$\begin{aligned}\ln p(\boldsymbol{X};\boldsymbol{\theta}) &= \int \widehat{p}(\boldsymbol{Z}) \ln p(\boldsymbol{X};\boldsymbol{\theta})\, \mathrm{d}\boldsymbol{Z} \\ &= \int \widehat{p}(\boldsymbol{Z}) \ln\left(\frac{p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta})}{\widehat{p}(\boldsymbol{Z})} \frac{\widehat{p}(\boldsymbol{Z})}{p(\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta})}\right) \mathrm{d}\boldsymbol{Z} \\ &= \underbrace{\int \widehat{p}(\boldsymbol{Z}) \ln p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta})\, \mathrm{d}\boldsymbol{Z}}_{\mathbb{E}_{\widehat{p}}\{\ln p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta})\}} \underbrace{- \int \widehat{p}(\boldsymbol{Z}) \ln \widehat{p}(\boldsymbol{Z})\, \mathrm{d}\boldsymbol{Z}}_{\text{entropy, } H(\widehat{p})} + \underbrace{\int \widehat{p}(\boldsymbol{Z}) \ln \frac{\widehat{p}(\boldsymbol{Z})}{p(\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta})}\, \mathrm{d}\boldsymbol{Z}}_{\text{KL divergence, } \geq 0}\end{aligned}$$

  and thus we have a lower bound on the log-likelihood:

$$\ln p(\boldsymbol{X};\boldsymbol{\theta}) \geq \mathbb{E}_{\widehat{p}}\{\ln p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta})\} + H(\widehat{p}) \triangleq \mathcal{L}(\widehat{p};\boldsymbol{\theta})$$

- The EM algorithm iterates the following steps:
  - E) tighten $\mathcal{L}(\widehat{p};\boldsymbol{\theta})$ through choice of $\widehat{p}$
  - M) maximize $\mathcal{L}(\widehat{p};\boldsymbol{\theta})$ through choice of $\boldsymbol{\theta}$



EM explained: Iterative maximization of lower bound

- Iteratively tightening and maximizing a lower bound is called majorization-minimization (MM). So, EM is a special case of MM.
- For EM, the bound tightening goes as follows:
  - At iteration t, we have
    $$\ln p(\boldsymbol{X};\boldsymbol{\theta}^{(t)}) = \underbrace{\mathbb{E}_{\widehat{p}}\{\ln p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta}^{(t)})\} + H(\widehat{p})}_{\mathcal{L}(\widehat{p};\boldsymbol{\theta}^{(t)})} + \underbrace{\int \widehat{p}(\boldsymbol{Z}) \ln \frac{\widehat{p}(\boldsymbol{Z})}{p(\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta}^{(t)})}\, \mathrm{d}\boldsymbol{Z}}_{\text{KL},\ \geq 0}$$
  - The tightest bound occurs when KL $= 0$, i.e., when $\widehat{p}(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta}^{(t)})$
  - This is exactly the choice used by EM at iteration t
- For EM, the lower-bound maximization goes as follows:
  - At iteration t, we have
    $$\mathcal{L}(\widehat{p};\boldsymbol{\theta}) = \mathbb{E}_{\widehat{p}}\{\ln p(\boldsymbol{Z},\boldsymbol{X};\boldsymbol{\theta})\} + H(\widehat{p}) \quad \text{with} \quad \widehat{p}(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X};\boldsymbol{\theta}^{(t)})$$
  - EM maximizes the first term with respect to $\boldsymbol{\theta}$, since 2nd term is invariant to $\boldsymbol{\theta}$

Application of EM to GMM fitting: E-step

- As hidden variables, we choose $\kappa_i \in \{1, \ldots, K\}$ for each $\boldsymbol{x}_i$, i.e., $\boldsymbol{Z} = [\kappa_1, \ldots, \kappa_n]$
- At iteration t, the E-step computes

$$\begin{aligned}
\mathcal{Q}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(t)}) &= \int p(\boldsymbol{\kappa} \,|\, \boldsymbol{X}; \boldsymbol{\theta}^{(t)}) \ln \overbrace{p(\boldsymbol{X}, \boldsymbol{\kappa}; \boldsymbol{\theta})}^{\prod_i p(\boldsymbol{x}_i, \kappa_i; \boldsymbol{\theta})} \, \mathrm{d}\boldsymbol{\kappa} \\
&= \sum_i \int p(\kappa_i \,|\, \boldsymbol{x}_i; \boldsymbol{\theta}^{(t)}) \ln p(\boldsymbol{x}_i, \kappa_i; \boldsymbol{\theta}) \, \mathrm{d}\kappa_i \\
&= \sum_i \sum_k \underbrace{\Pr\{\kappa_i = k \,|\, \boldsymbol{x}_i; \boldsymbol{\theta}^{(t)}\}}_{\triangleq \gamma_{ki}^{(t)}} \ln \underbrace{p(\boldsymbol{x}_i, \kappa_i = k; \boldsymbol{\theta})}_{p(\boldsymbol{x}_i | \kappa_i = k; \boldsymbol{\theta}) \Pr\{\kappa_i = k; \boldsymbol{\theta}\}}
\end{aligned}$$

where

$$\gamma_{ki}^{(t)} = \frac{\gamma_k^{(t)} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k^{(t)}, \boldsymbol{Q}_k^{(t)})}{\sum_{k'} \gamma_{k'}^{(t)} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{k'}^{(t)}, \boldsymbol{Q}_{k'}^{(t)})} \quad \text{can be computed } \forall k, i$$

$$\begin{aligned}
p(\boldsymbol{x}_i | \kappa_i = k; \boldsymbol{\theta}) &= \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k, \boldsymbol{Q}_k) \\
\Pr\{\kappa_i = k; \boldsymbol{\theta}\} &= \gamma_k
\end{aligned}$$

Application of EM to GMM fitting: M-step

- At iteration t, the M-step computes

$$\begin{aligned}\boldsymbol{\theta}^{(t+1)} &= \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta};\boldsymbol{\theta}^{(t)}) \\ &= \arg\max_{\boldsymbol{\theta}} \Big\{ \sum_{i,k} \gamma_{ki}^{(t)} \ln \gamma_k + \sum_{i,k} \gamma_{ki}^{(t)} \ln \mathcal{N}(\boldsymbol{x}_i;\boldsymbol{\mu}_k,\boldsymbol{Q}_k) \Big\}\end{aligned}$$

- To maximize over γ_k s.t. $\sum_k \gamma_k = 1$, we zero the gradient of the Lagrangian:

$$\begin{aligned} 0 &= \frac{\partial}{\partial \gamma_k}\Big\{ \sum_{i,k'} \gamma_{k'i}^{(t)} \ln \gamma_{k'} + \lambda\Big(1 - \sum_{k'} \gamma_{k'}\Big)\Big\} = \frac{1}{\gamma_k}\sum_i \gamma_{ki}^{(t)} - \lambda \\ \Rightarrow 0 &= \sum_i \gamma_{ki}^{(t)} - \lambda\gamma_k \qquad (1) \\ \Rightarrow 0 &= \sum_i \sum_k \gamma_{ki}^{(t)} - \lambda \sum_k \gamma_k = \sum_i 1 - \lambda = n - \lambda \\ \Rightarrow \lambda &= n, \quad \text{and so now we know the value of the Lagrange multiplier } \lambda \end{aligned}$$

Application of EM to GMM fitting: M-step

- Solving for γ_k via (1) and plugging in λ, we find

$$\gamma_k = \frac{1}{\lambda}\sum_i \gamma_{ki}^{(t)} = \frac{1}{n}\sum_i \gamma_{ki}^{(t)}, \text{ which we use for } \gamma_k^{(t+1)}$$

- To maximize over $\boldsymbol{\mu}_k$, we zero the gradient of the cost w.r.t. $\boldsymbol{\mu}_k$:

$$\begin{aligned}
\mathbf{0} &= \nabla_{\boldsymbol{\mu}_k}\left\{\sum_{i,k'} \gamma_{k'i}^{(t)} \ln \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{k'}, \boldsymbol{Q}_{k'})\right\} \\
&= \sum_i \gamma_{ki}^{(t)} \nabla_{\boldsymbol{\mu}_k}\left\{-\frac{1}{2}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^\mathsf{T}\boldsymbol{Q}_k^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu}_k) + \text{const}\right\} \\
&= \sum_i \gamma_{ki}^{(t)} \boldsymbol{Q}_k^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu}_k) = \boldsymbol{Q}_k^{-1}\left(\sum_i \gamma_{ki}^{(t)}\boldsymbol{x}_i - \boldsymbol{\mu}_k \sum_i \gamma_{ki}^{(t)}\right) \\
\Rightarrow \boldsymbol{\mu}_k &= \frac{\sum_i \gamma_{ki}^{(t)}\boldsymbol{x}_i}{\sum_i \gamma_{ki}^{(t)}}, \text{ which we use for } \boldsymbol{\mu}_k^{(t+1)}
\end{aligned}$$

- Finally, $\boldsymbol{Q}_k$ can be optimized in a similar manner, giving $\boldsymbol{Q}_k^{(t+1)}$

Application of EM to GMM fitting: Summary

- Initialize $\gamma_k^{(0)}, \boldsymbol{\mu}_k^{(0)}, \boldsymbol{Q}_k^{(0)}$ and repeat for $t = 0, 1, 2 \dots$

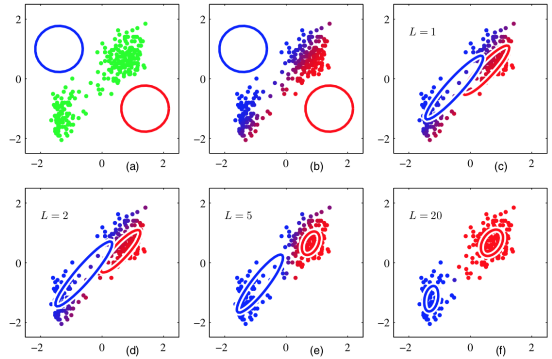
$$\begin{aligned}
\forall k, i: \quad \gamma_{ki}^{(t)} &= \frac{\gamma_k^{(t)} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k^{(t)}, \boldsymbol{Q}_k^{(t)})}{\sum_{k'} \gamma_{k'}^{(t)} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{k'}^{(t)}, \boldsymbol{Q}_{k'}^{(t)})} \\
\forall k: \quad \gamma_k^{(t+1)} &= \tfrac{1}{n} \textstyle\sum_{i=1}^n \gamma_{ki}^{(t)} \\
\forall k: \quad \boldsymbol{\mu}_k^{(t+1)} &= \tfrac{1}{n} \textstyle\sum_{i=1}^n \frac{\gamma_{ki}^{(t)}}{\gamma_k^{(t+1)}} \boldsymbol{x}_i \\
\forall k: \quad \boldsymbol{Q}_k^{(t+1)} &= \tfrac{1}{n} \textstyle\sum_{i=1}^n \frac{\gamma_{ki}^{(t)}}{\gamma_k^{(t+1)}} (\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)})(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)})^\mathsf{T}
\end{aligned}$$

- For the initialization, it is common to use k-means++:
  - set $\gamma_k^{(0)}$ to the fraction of samples that k-means++ assigned to k
  - set $\boldsymbol{\mu}_k^{(0)}, \boldsymbol{Q}_k^{(0)}$ to mean & covariance of samples that k-means++ assigned to k
- When the dimension d is large, it is typical to approximate $\boldsymbol{Q}_k$ as diagonal

Application of EM to GMM fitting: Example

Example of EM algorithm fitting a Gaussian mixture with $K = 2$ components

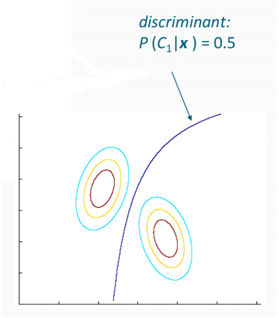
- Ellipses show a contour of $\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k^{(t)}, \boldsymbol{Q}_k^{(t)})$ for $k = 1, 2$
- Soft assignments $\gamma_{ki}^{(t)}$ shown by dot color (from red to blue)
- In plots, iteration t is denoted by "L"



Bishop, *Pattern Recognition and Machine Learning*, 2006

Comparison of EM-GMM to k-means

- EM computes soft assignments $\Pr\{\kappa_i = k\}$, while k-means computes hard assignments $\widehat{\kappa}(\boldsymbol{x}_i)$
- EM estimates covariances $\boldsymbol{Q}_k$, while k-means implicitly uses $\boldsymbol{Q}_k = \epsilon \boldsymbol{I}\ \forall k$ with vanishingly small ϵ
  - EM uses piecewise curved decision boundaries
  - k-means uses piecewise linear boundaries
- EM estimates weights $\gamma_k \in (0,1)$, while k-means implicitly uses $\gamma_k = \frac{1}{K}\ \forall k$
- EM is more computationally expensive than k-means



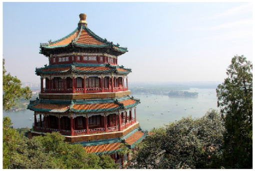
- Both can get stuck in local minima; both benefit from a good initialization
- Both implemented in sklearn, e.g.,

```
GMM = GaussianMixture(n_components=n_colors, covariance_type = 'diag',
                      max_iter=100, random_state=0, init_params = 'kmeans')
GMM.fit(image_array_sample)
GMM_labels = GMM.predict(image_array)
```

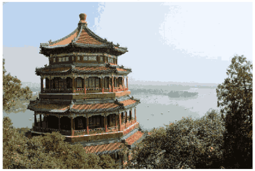
Demo: Color quantization via clustering

- Standard "true color" image
  - $256 = 2^8$ possibilities each for R, G, B
  - 24 bits per pixel
  - $2^{24} = 16\,777\,216$ unique possibilities in color palette
- Goal: Reduce color palette down to 16 possibilities
  - 4 bits per pixel
  - Question: What are the $2^4 = 16$ best colors?
- Idea: Treat as a clustering problem:
  - $d = 3$ features, $K = 16$ centroids
  - learn centroids from $n = 1000$ random pixels
  - then quantize all $273\,280$ pixels to these centroids
- We compare EM-GMM and k-means++ on the right
  - EM-GMM better preserves fine details

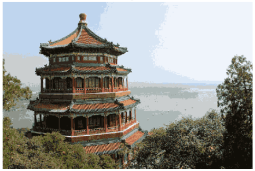
Original image (96,615 colors)



Quantized image (GMM)



Quantized image (K-Means)

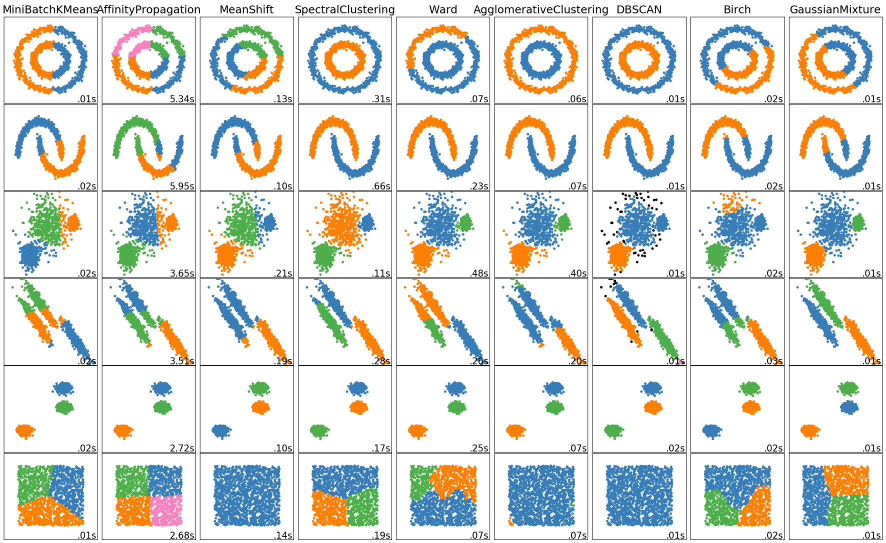


Outline

Model-order selection

- Both k-means and EM-GMM require the number of components K as input
- Various other clustering methods learn K automatically, e.g.,
  - Dirichlet process mixture model
  - mean-shift
  - affinity propagation
  - many others . . . see examples on next page
- Another important question is: What features should we use for clustering?
  - Can imagine using non-linear feature transformations, e.g., a kernel. This leads to the spectral clustering method . . . see example on next page
  - Or could try to learn a non-linear feature transformation using a neural network. This is sometimes called deep clustering and is an active area of research

Other clustering methods in `sklearn.cluster`



Learning objectives

- Understand the k-means clustering objective and Lloyd's algorithm
- Understand term-document matrices and TF-IDF scores for text-mining
- Understand NMF, its relation to PCA and application to clustering
- Understand GMMs and their application to clustering
- Understand the EM algorithm and its application to GMM parameter fitting