Clustering / Unsupervised Methods

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Introduction

- Until now, we've assumed our training samples are "labeled" by their category membership.
- Methods that use labeled samples are said to be *supervised*; otherwise, they're said to be *unsupervised*.
- However:
  - Why would one even be interested in learning with unlabeled samples?
  - Is it even possible in principle to learn anything of value from unlabeled samples?

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   - Train a classifier on a small set of samples, then tune it up to make it run without supervision on a large, unlabeled set.
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4. To find features that will then be useful for categorization.
5. To gain insight into the nature or structure of the data during the early stages of an investigation.

Data Clustering

Source: A. K. Jain and R. C. Dubes. Alg. for Clustering Data, Prentiice Hall, 1988.

- What is data clustering?
  - Grouping of objects into meaningful categories
  - Given a **representation** of N objects, find k clusters based on a measure of **similarity**.

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  - Natural Classification: degree of similarity among forms.
  - Data exploration: discover underlying structure, generate hypotheses, detect anomalies.
  - Compression: for organizing data.
  - Applications: can be used by any scientific field that collects data!

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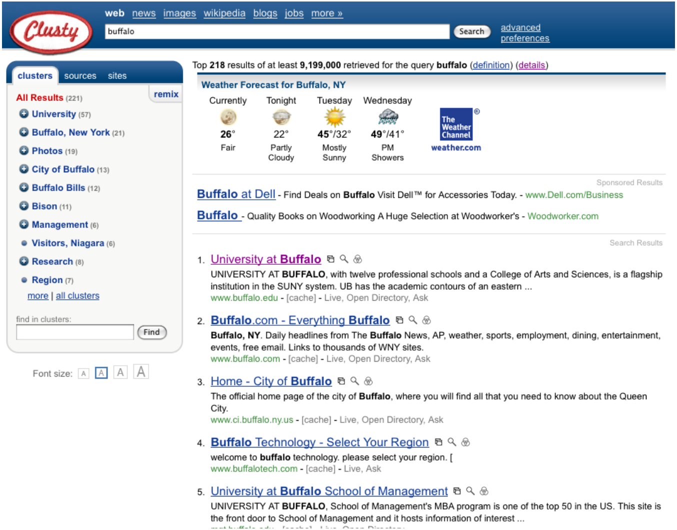
  - Applications: can be used by any scientific field that collects data!
- Google Scholar: 1500 clustering papers in 2007 alone!

E.g.: Structure Discovering via Clustering

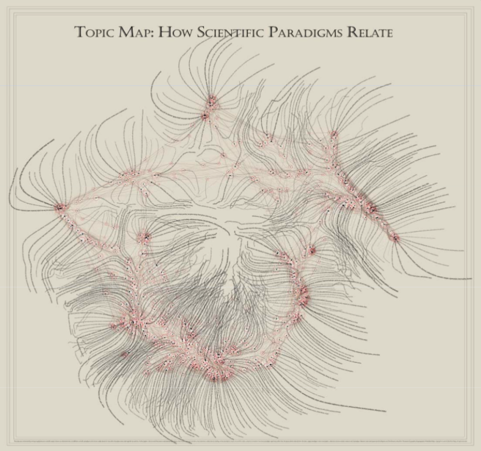
Source: http://clusty.com



E.g.: Topic Discovery

Source: Map of Science, Nature, 2006

- 800,000 scientific papers clustered into 776 topics based on how often the papers were cited together by authors of other papers



Data Clustering - Formal Definition

- Given a set of N unlabeled examples $D = x_1, x_2, ..., x_N$ in a d-dimensional feature space, D is partitioned into a number of disjoint subsets D_j's:

$$D = \cup_{j=1}^{k} D_j \quad \text{where } D_i \cap D_j = \emptyset, i \neq j \ , \tag{1}$$

  where the points in each subset are similar to each other according to a given criterion ϕ.

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  where the points in each subset are similar to each other according to a given criterion ϕ.
- A partition is denoted by

$$\pi = (D_1, D_2, ..., D_k) \tag{2}$$

  and the problem of data clustering is thus formulated as

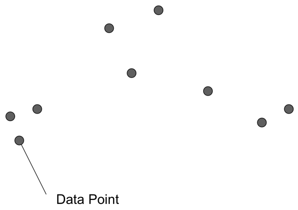
$$\pi^* = \underset{\pi}{\operatorname{argmin}} \ f(\pi) \ , \tag{3}$$

  where $f(\cdot)$ is formulated according to ϕ.

k-Means Clustering

Source: D. Aurthor and S. Vassilvitskii. k-Means++: The Advantages of Careful Seeding

- Randomly initialize $\mu_1, \mu_2, ..., \mu_c$
- Repeat until no change in μ_i:
  - Classify N samples according to nearest μ_i
  - Recompute μ_i



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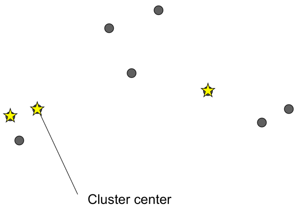

First choose *k* arbitrary centers

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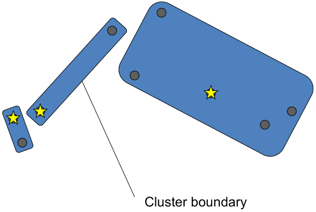

Assign points to closest centers

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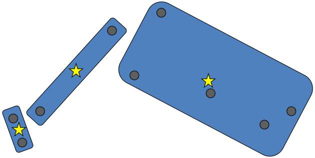

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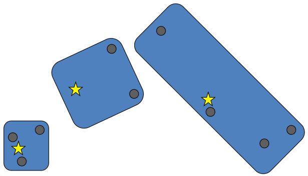

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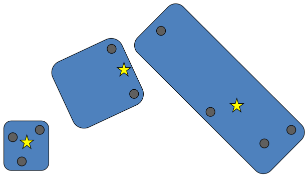

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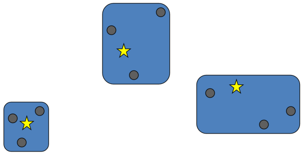

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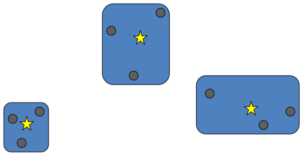

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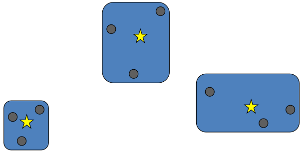

Points already assigned to nearest centers: Algorithm ends

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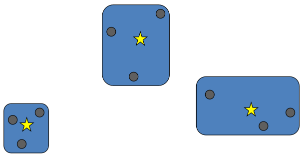

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k-Means++ Clustering

Source: D. Aurthor and S. Vassilvitskii. k-Means++: The Advantages of Careful Seeding

- Choose starting centers iteratively.
- Let $D(x)$ be the distance from x to the nearest existing center, take x as new center with probability $\propto D(x)^2$.
- Repeat until no change in μ_i:
  - Classify N samples according to nearest μ_i
  - Recompute μ_i
- (refer to the slides by D. Aurthor and S. Vassolvitskii for details)

User's Dilemma

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

1. What is a cluster?
2. How to define pair-wise similarity?

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2. How to define pair-wise similarity?
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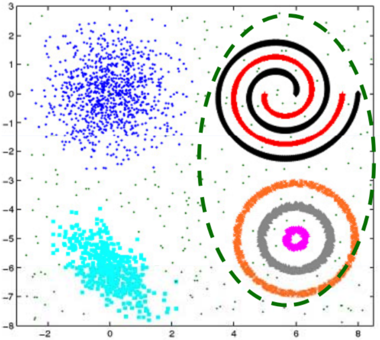
4. How many clusters?
5. Which clustering method?
6. Are the discovered clusters and partition valid?
7. Does the data have any clustering tendency?

Cluster Similarity?

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

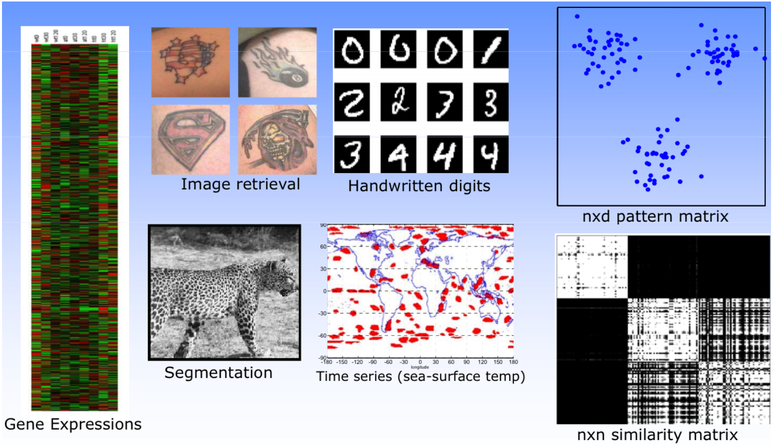
- Compact Clusters
  - Within-cluster **distance** $<$ between-cluster connectivity
- Connected Clusters
  - Within-cluster **connectivity** $>$ between-cluster connectivity
- Ideal cluster: **compact** and **isolated**.



Representation (features)?

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

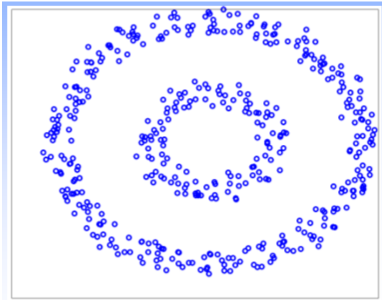
- There's no universal representation; they're domain dependent.



Good Representation

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

- A good representation leads to compact and isolated clusters.



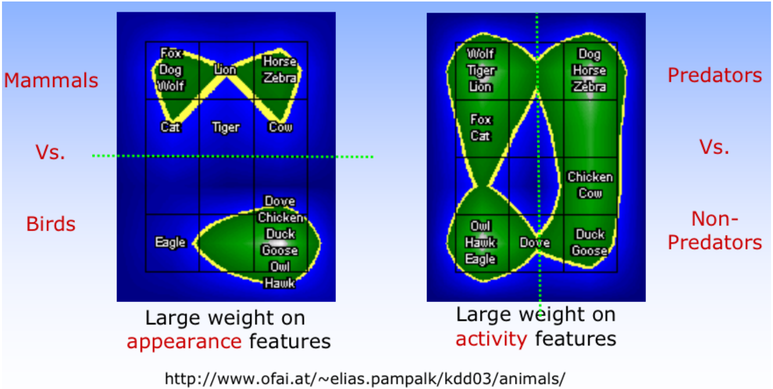
Points in given 2D space

Representation based on eigenvectors of RBF kernel

How do we weigh the features?

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

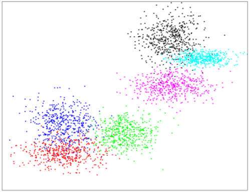
- Two different meaningful groupings produced by different weighting schemes.



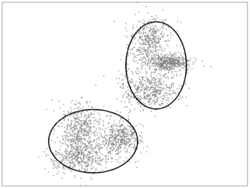
How do we decide the Number of Clusters?

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

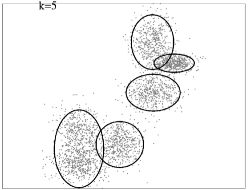
- The samples are generated by 6 independent classes, yet:



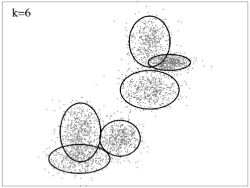
ground truth



$k = 2$



$k = 5$

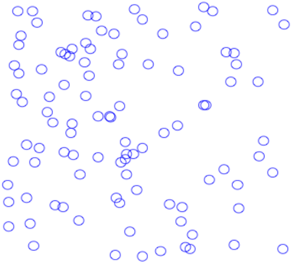


$k = 6$

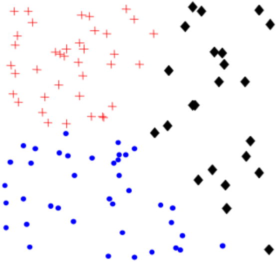
Cluster Validity

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

- Clustering algorithms find clusters, even if there are no **natural** clusters in the data.



100 2D uniform data points

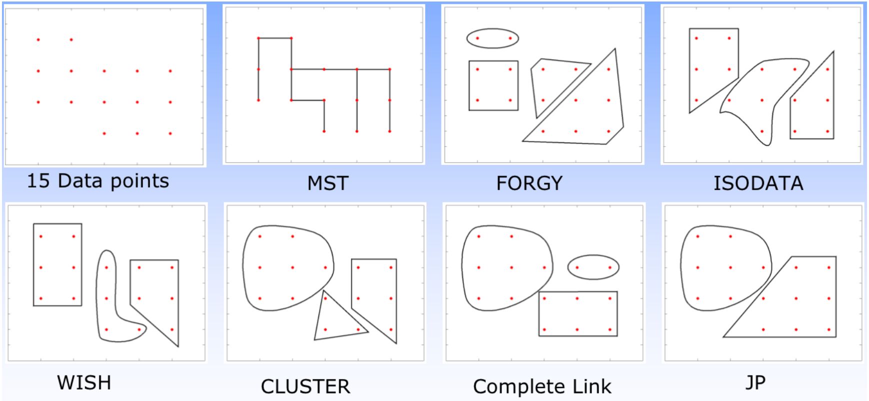


k-Means with k=3

Comparing Clustering Methods

Source: R. Dubes and A. K. Jain, Clustering Techniques: User's Dilemma, PR 1976

- Which clustering algorithm is the best?



There's no best Clustering Algorithm!

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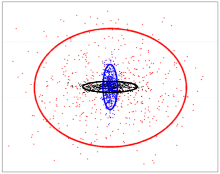
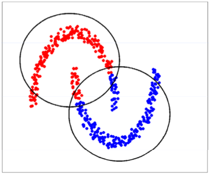
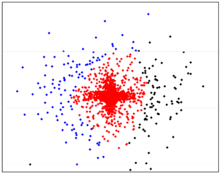
- Each algorithm imposes a structure on data.
- Good fit between model and data $\Rightarrow$ success.



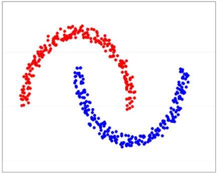
GMM; k=3



GMM; k=2



Spectral; k=3



Spectral; k=2

Gaussian Mixture Models

- Recall the Gaussian distribution:

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right] \quad (4)$$

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- The Gaussian mixture is a **linear superposition of Gaussians** in the form:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \ . \quad (5)$$

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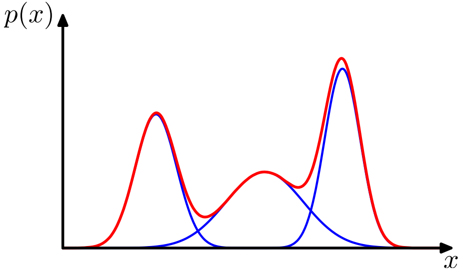
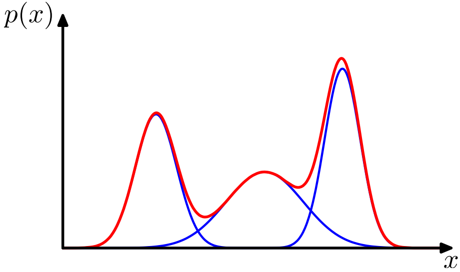
- The π_k are non-negative scalars called **mixing coefficients** and they govern the relative importance between the various Gaussians in the mixture density. $\sum_k \pi_k = 1$.


$p(x)$
x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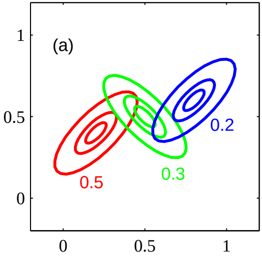
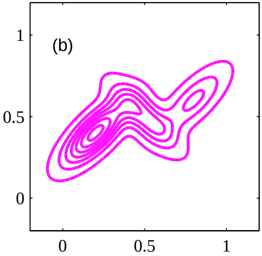
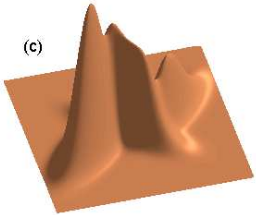

(a)
1
0.5
0
0
0.5
1
0.5
0.3
0.2


(b)
1
0.5
0
0
0.5
1


(c)

Introducing Latent Variables

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$$\sum_k z_k = 1 \tag{7}$$

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- $\mathbf{z}$ has a 1-of-K representation such that a particular element z_k is 1 and all of the others are zero. Hence:

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$$\sum_k z_k = 1 \tag{7}$$

- The marginal distribution over $\mathbf{z}$ is specified in terms of the mixing coefficients:

$$p(z_k = 1) = \pi_k \tag{8}$$

And, recall, $0 \leq \pi_k \leq 1$ and $\sum_k \pi_k = 1$.

- Since $\mathbf{z}$ has a 1-of-K representation, we can also write this distribution as

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- The conditional distribution of $\mathbf{x}$ given $\mathbf{z}$ is a Gaussian:

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{10}$$

or

$$p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k} \tag{11}$$

- We are interested in the marginal distribution of $\mathbf{x}$:

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- If we have N observations $\mathbf{x}_1, \ldots, \mathbf{x}_N$, then because of our chosen representation, it follows that we have a latent variable $\mathbf{z}_n$ for each observed data point $\mathbf{x}_n$.

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- View π_k as the prior probability of $z_k = 1$ and the quantity $\gamma(z_k)$ as the corresponding posterior probability once we have observed $\mathbf{x}$.
- $\gamma(z_k)$ can also be viewed as the responsibility that component k takes for explaining the observation $\mathbf{x}$.

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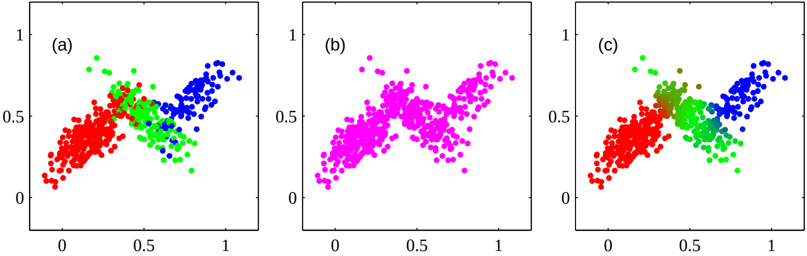

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- Ultimately, we want to find the values of the parameters $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$ that maximize this function.

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- However, maximizing the log-likelihood terms for GMMs is much more complicated than for the case of a single Gaussian. Why?
- The difficulty arises from the sum over k inside of the log-term. The log function no longer acts directly on the Gaussian, and no closed-form solution is available.

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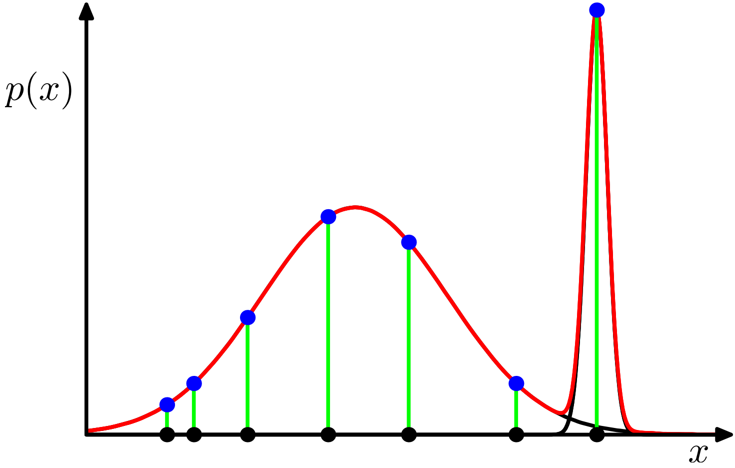
- Consider the limit $\sigma_j \to 0$ to see that this term goes to infinity and hence the log-likelihood will also go to infinity.
- **Thus, the maximization of the log-likelihood function is not a well posed problem because such a singularity will occur whenever one of the components collapses to a single, specific data point.**


$p(x)$
x

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- Recall the conditions that must be satisfied at a maximum of the likelihood function.
- For the mean $\boldsymbol{\mu}_k$, setting the derivatives of $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ w.r.t. $\boldsymbol{\mu}_k$ to zero yields

$$0 = -\sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \boldsymbol{\Sigma}_k (\mathbf{x}_n - \boldsymbol{\mu}_k) \tag{20}$$

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- Note the natural appearance of the responsibility terms on the RHS.

- Multiplying by $\boldsymbol{\Sigma}_k^{-1}$, which we assume is non-singular, gives

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- We find a similar result for the covariance matrix:

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(x_n - \boldsymbol{\mu}_k)(x_n - \boldsymbol{\mu}_k)^{\mathsf{T}} \ . \tag{24}$$

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- Eliminate λ and rearrange to obtain:

$$\pi_k = \frac{N_k}{N} \tag{28}$$

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$$\gamma(z_k) \doteq p(z_k = 1|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

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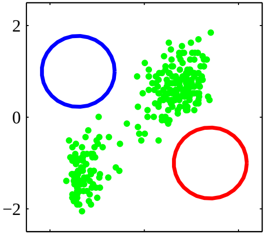
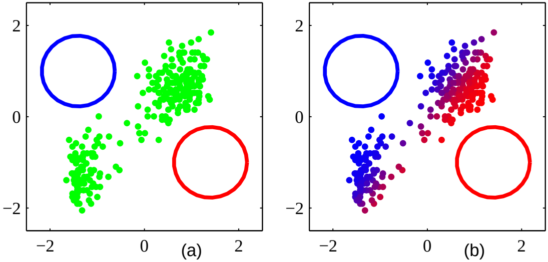
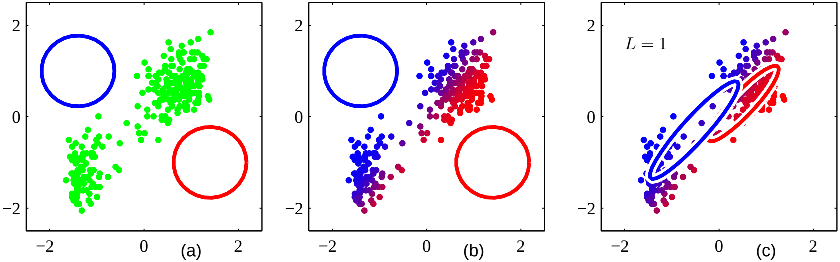
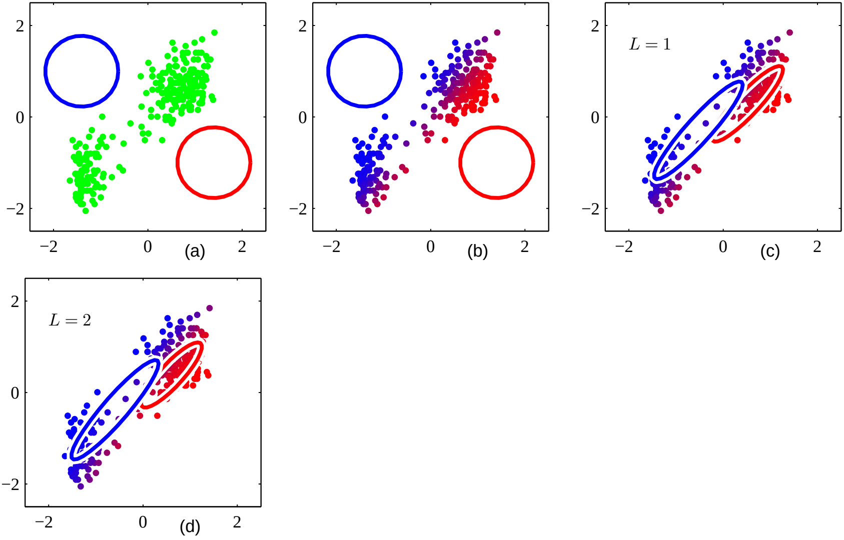
- But, these results do suggest an iterative scheme for finding a solution to the maximum likelihood problem.
  1. Chooce some initial values for the parameters, $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$.
  2. Use the current parameters estimates to compute the posteriors on the latent terms, i.e., the responsibilities.
  3. Use the responsibilities to update the estimates of the parameters.
  4. Repeat 2 and 3 until convergence.

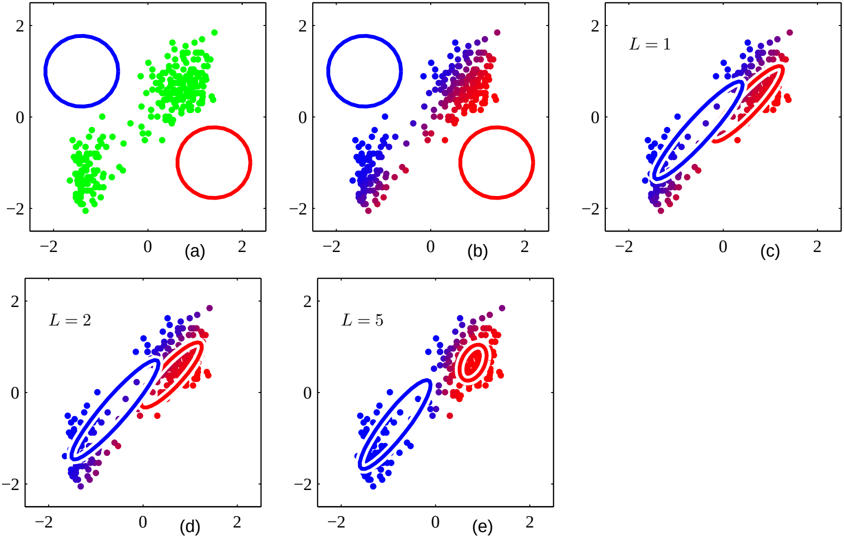


(a)

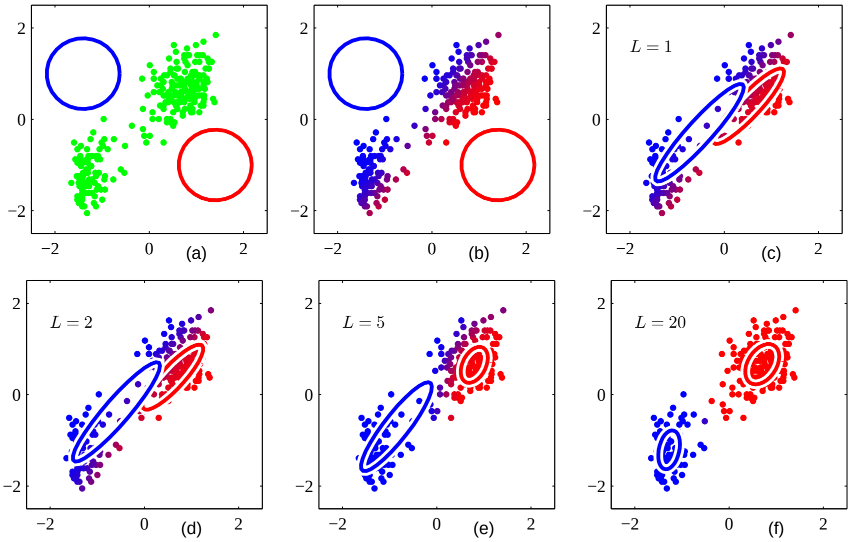

2
0
−2
−2
0
(a)
2
2
0
−2
−2
0
(b)
2


2
0
−2
−2
0
2
(a)
2
0
−2
−2
0
2
(b)
2
0
−2
−2
0
2
(c)
$L = 1$


2
0
−2
−2
0
2
(a)
2
0
−2
−2
0
2
(b)
$L = 1$
2
0
−2
−2
0
2
(c)
$L = 2$
2
0
−2
−2
0
2
(d)



2
0
−2
−2
0
2
(a)
(b)
L = 1
(c)
L = 2
(d)
L = 5
(e)


L = 1
L = 2
L = 5
L = 20
(a)
(b)
(c)
(d)
(e)
(f)

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- Care must be taken to avoid singularities in the MLE solution.
- There will generally be multiple local maxima of the likelihood function and EM is not guaranteed to find the largest of these.

Given a GMM, the goal is to maximize the likelihood function with respect to the parameters (the means, the covarianes, and the mixing coefficients).

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Given a GMM, the goal is to maximize the likelihood function with respect to the parameters (the means, the covarianes, and the mixing coefficients).

1. Initialize the means, $\boldsymbol{\mu}_k$, the covariances, $\boldsymbol{\Sigma}_k$, and mixing coefficients, $\boldsymbol{\pi}_k$. Evaluate the initial value of the log-likelihood.
2. **E-Step** Evaluate the responsibilities using the current parameter values:
$$\gamma(z_k) = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$
3. **M-Step** Update the parameters using the current responsibilities
$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \tag{29}$$
$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\mathsf{T}} \tag{30}$$
$$\pi_k^{\text{new}} = \frac{N_k}{N} \tag{31}$$
where
$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}) \tag{32}$$

4. Evaluate the log-likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu}^{\text{new}}, \boldsymbol{\Sigma}^{\text{new}}, \boldsymbol{\pi}^{\text{new}}) = \sum_{n=1}^{N} \ln \left[\sum_{k=1}^{K} \pi_k^{\text{new}} \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k^{\text{new}}, \boldsymbol{\Sigma}_k^{\text{new}}\right) \right] \tag{33}$$

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5. Check for convergence of either the parameters of the log-likelihood. If the convergence is not satisfied, set the parameters:

$$\boldsymbol{\mu} = \boldsymbol{\mu}^{\text{new}} \tag{34}$$

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{\text{new}} \tag{35}$$

$$\boldsymbol{\pi} = \boldsymbol{\pi}^{\text{new}} \tag{36}$$

and goto step 2.

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    - Even if the joint distribution $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ belongs to the exponential family, the marginal $p(\mathbf{X}|\boldsymbol{\theta})$ typically does not.
- If, for each sample $\mathbf{x}_n$ we were given the value of the latent variable $\mathbf{z}_n$, then we would have a **complete** data set, $\{\mathbf{X}, \mathbf{Z}\}$, with which maximizing this likelihood term would be straightforward.

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$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) \tag{38}$$

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- Then, in the M-step, we revise the parameters to $\boldsymbol{\theta}^{\text{new}}$ by maximizing this function:

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- Note that the log acts directly on the joint distribution $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ and so the M-step maximization will likely be tractable.