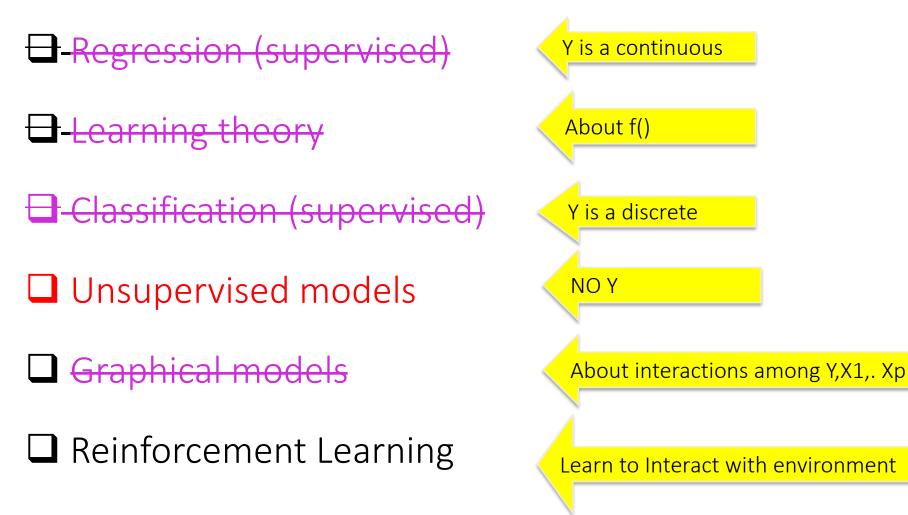
UVA CS 4774: Machine Learning

S5: Lecture 25 Extra: Unsupervised Clustering (III): Gaussian Mixture Model

Dr. Yanjun Qi

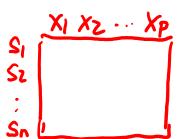
University of Virginia Department of Computer Science

Course Content Plan → Regarding Tasks

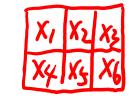


Course Content Plan → Regarding Data

Tabular / Matrix



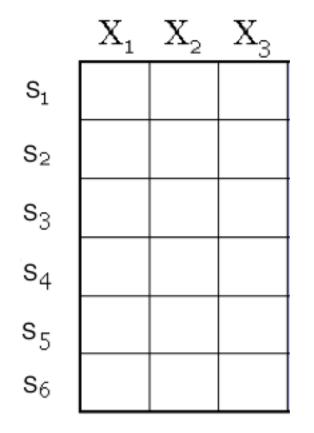
2D Grid Structured: Imaging



□ 1D Sequential Structured: Text

Graph Structured (Relational)

□ Set Structured / 3D /



An unlabeled Dataset X

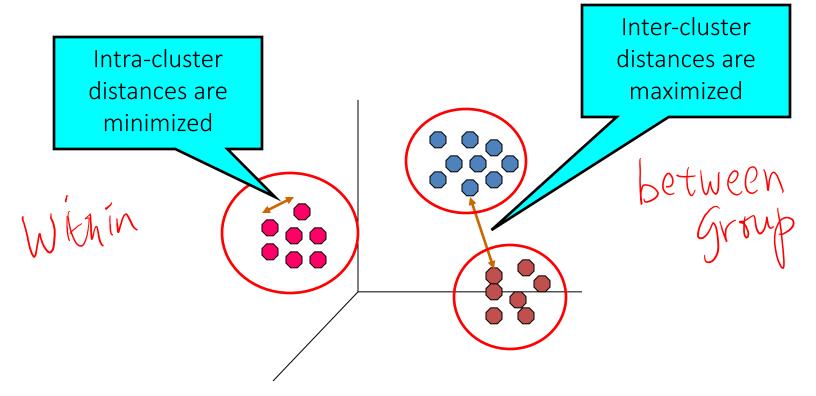
a data matrix of n observations on p variables $x_1, x_2, ..., x_p$

Unsupervised learning = learning from raw (unlabeled, unannotated, etc) data, as opposed to supervised data where a classification label of examples is given

- Data/points/instances/examples/samples/records: [rows]
- Features/attributes/dimensions/independent variables/covariates/predictors/regressors: [columns]

What is clustering?

 Find groups (clusters) of data points such that data points in a group will be similar (or related) to one another and different from (or unrelated to) the data points in other groups

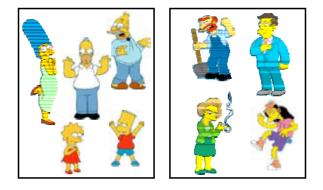


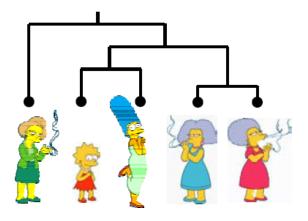
Roadmap: clustering

- Definition of "groupness"
- Definition of "similarity/distance"
- Representation for objects
- How many clusters?
- Clustering Algorithms
- Partitional algorithms
 - Hierarchical algorithms
 - Formal foundation and convergence

Clustering Algorithms

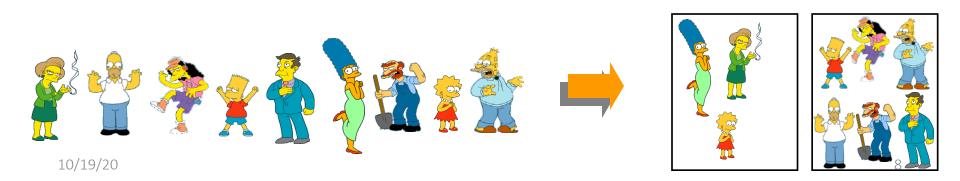
- Partitional algorithms
 - Usually start with a random (partial) partitioning
 - Refine it iteratively
 - K means clustering
 - Mixture-Model based clustering
- Hierarchical algorithms
 - Bottom-up, agglomerative
 - Top-down, divisive





(2) Partitional Clustering

- Nonhierarchical
- Construct a partition of n objects into a set of K clusters
- User has to specify the desired number of clusters K.



Other partitioning Methods

 Partitioning around medoids (PAM): instead of averages, use multidim medians as centroids (cluster "prototypes"). Dudoit and Freedland (2002).

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E.g.: SOM Used for Visualization

Islands of Music

Analysis, Organization, and Visualization of Music Archives

Islands of music (Pampalk et al., KDD' 03)

piece of music: member of a *music collection* and inhabitant of *islands of music*. Groups of similar pieces of music (also known as *genres*) like to gather around large mountains or small hills depending on the size of the group. Groups which are similar to each other like to live close together. Individuals which are not members of specific groups usually live near the beach and some very individualistic pieces might be found swimming in deep water.

islands of music: serve as graphical *user interface* to a music collection and are intended to help the user explore vast amounts of music in an efficient way. Islands of music are generated automatically based on *psychoacoustics models* and *self-organizing maps*. ¹¹

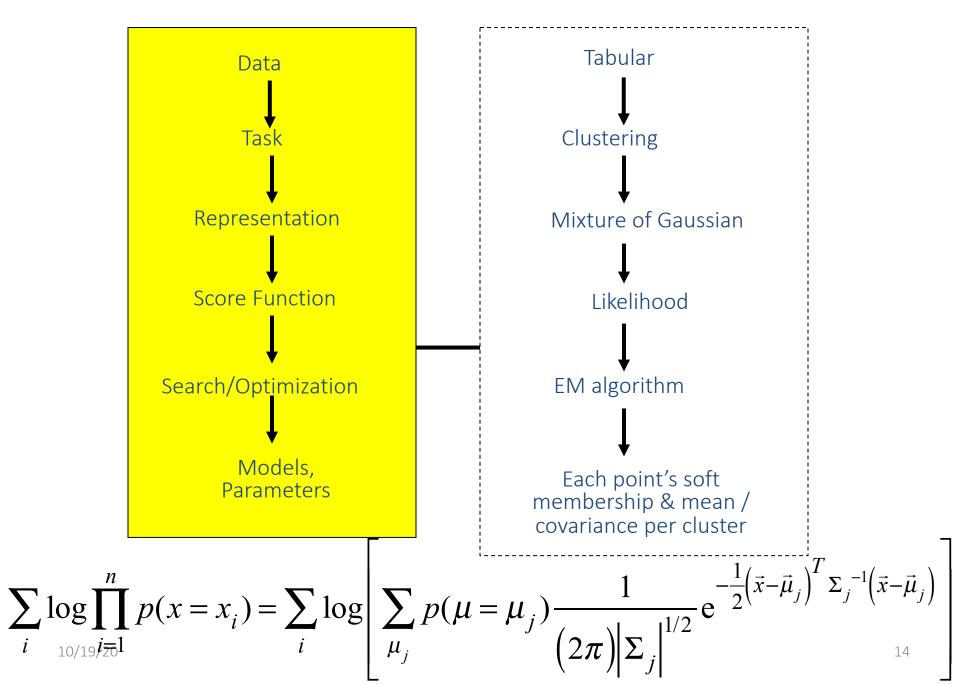
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- Fuzzy k-means: allow for a "gradation" of points between clusters; soft partitions. Gash and Eisen (2002).

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- Fuzzy k-means: allow for a "gradation" of points between clusters; soft partitions. Gash and Eisen (2002).
 - Mixture-based clustering: implemented through an EM (Expectation-Maximization)algorithm. This provides soft partitioning, and allows for modeling of cluster centroids and shapes. (Yeung et al. (2001), McLachlan et al. (2002))



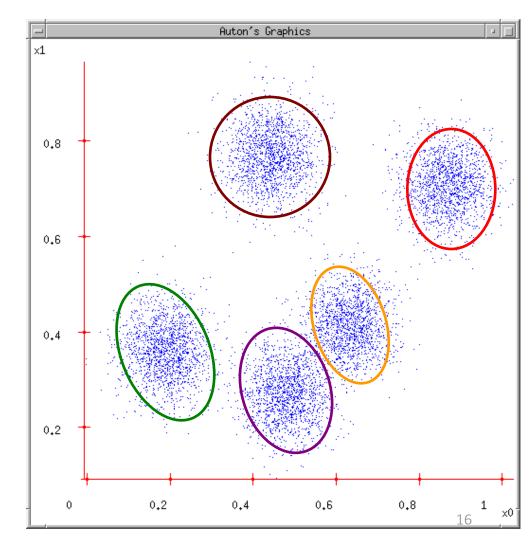


Partitional : Gaussian Mixture Model

- 1. Review of Gaussian Distribution
- 2. GMM for clustering : basic algorithm
- 3. GMM connecting to K-means
- 4. Problems of GMM and K-means

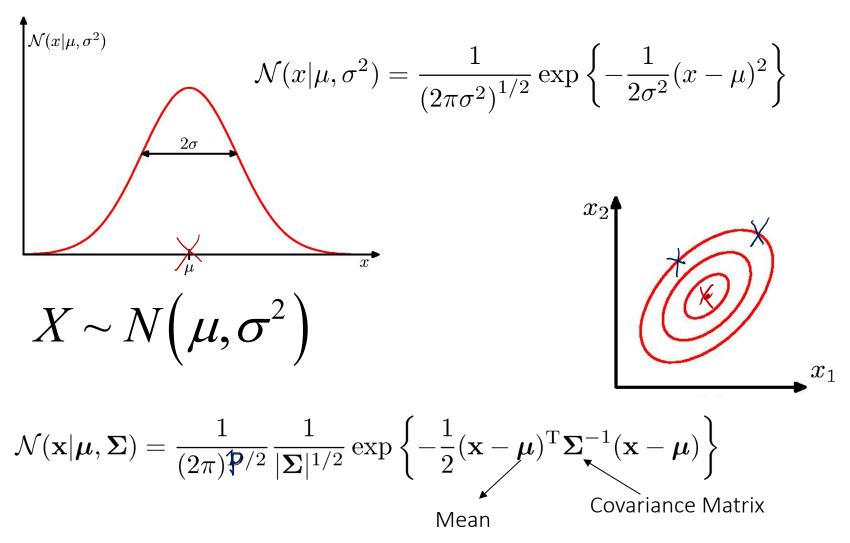
A Gaussian Mixture Model for Clustering

- Assume that data are generated from a mixture of Gaussian distributions
- For each Gaussian distribution
 - Center: μ_{j}
 - covariance: \sum_{j}
- For each data point
 - Determine membership
 - z_{ij} : if x_i belongs to j-th cluster



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Gaussian Distribution

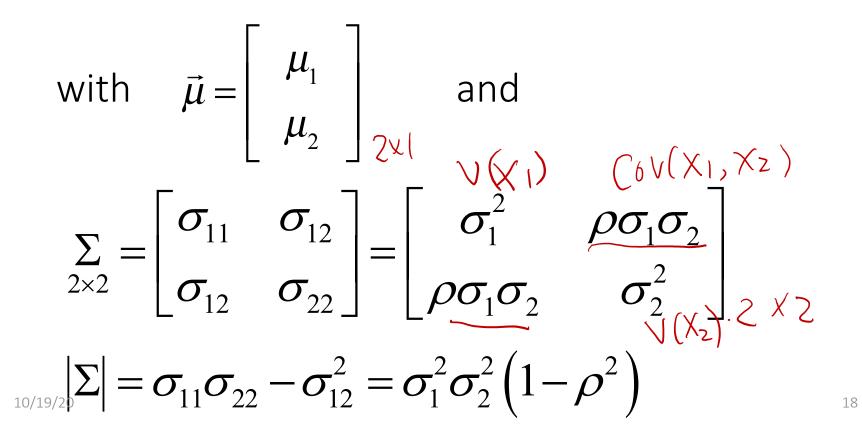


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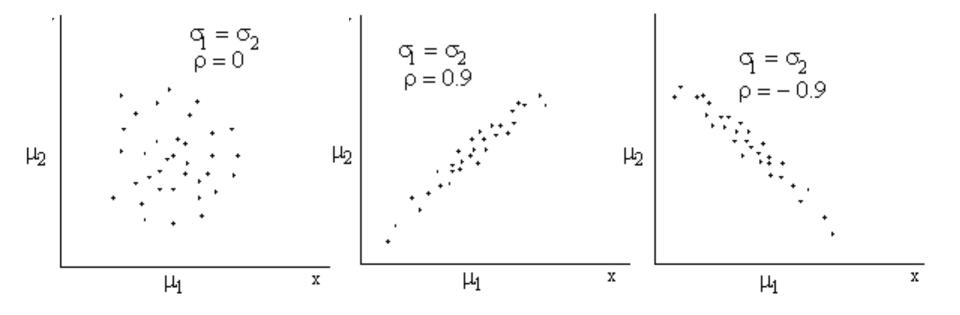
Courtesy: http://research.microsoft.com/~cmbishop/PRML/index.htm

Example: the Bivariate Normal distribution

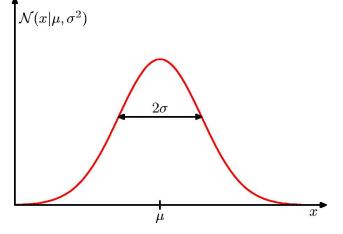
$$p(\vec{x}) = f(x_1, x_2) = \frac{1}{(2\pi)|\Sigma|^{1/2}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu})^T \Sigma^{-1}(\vec{x} - \vec{\mu})}$$



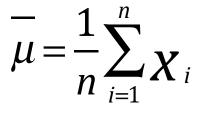
Scatter Plots of data from the bivariate Normal distribution



How to Estimate Gaussian: MLE



• In the 1D Gaussian case, we simply set the mean and the variance to the sample mean and the sample variance:



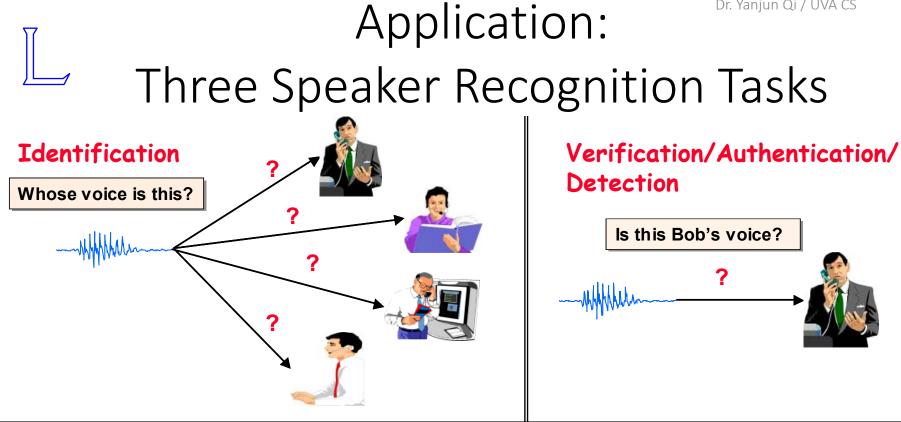
$$\overline{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \mu)^2$$

-2

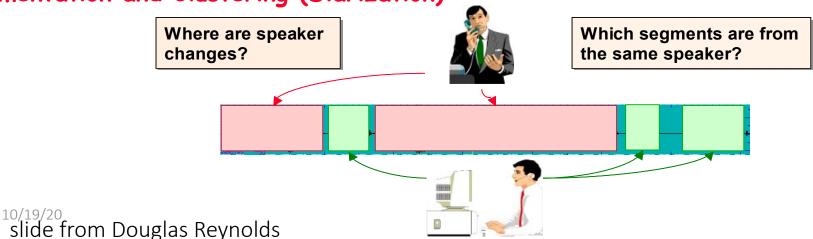
The p-multivariate Normal distribution € { 1, 2, ..., \$ $< X_1, X_2, \cdots, X_p > \sim N(\overline{\mu}, \Sigma)$ $\mathcal{M}_{v} = \frac{1}{N} \sum_{j=1}^{N} \frac{1}{j}$ $\overline{\mathcal{M}} = \begin{bmatrix} \mathcal{N}_1 \\ \mathcal{N}_2 \end{bmatrix}$ NIP -Sahr

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Segmentation and Clustering (Diarization)

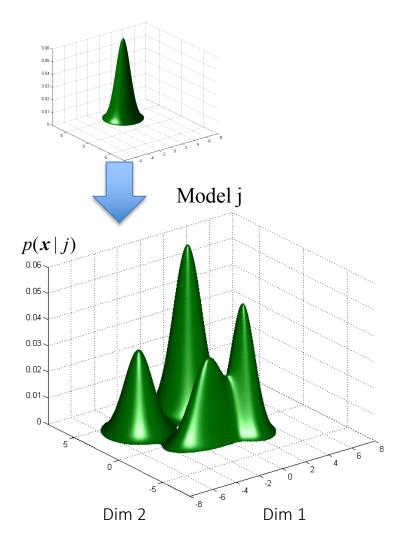


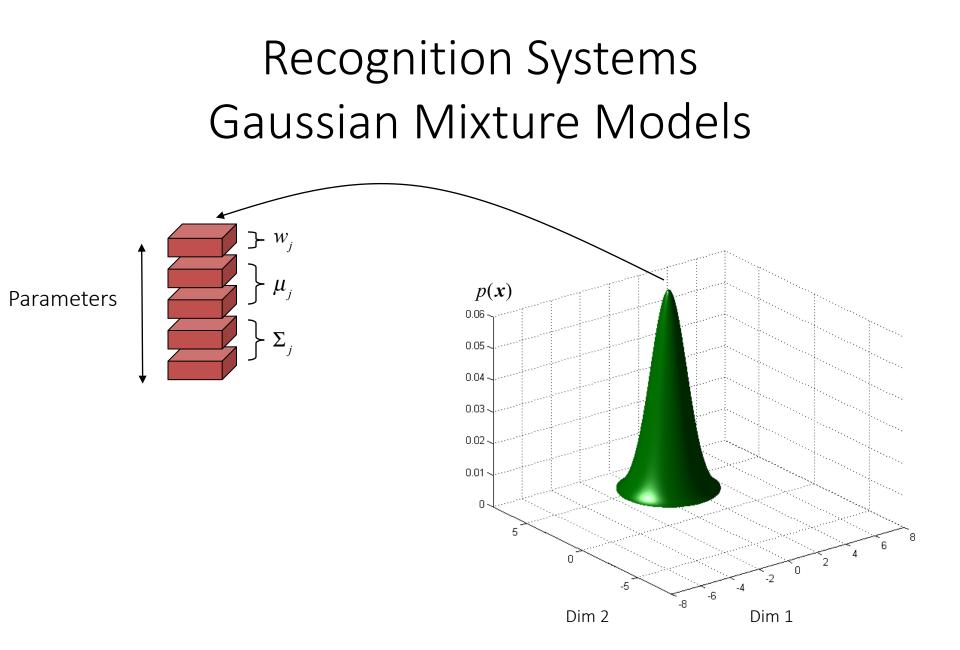
Application : GMMs for speaker recognition

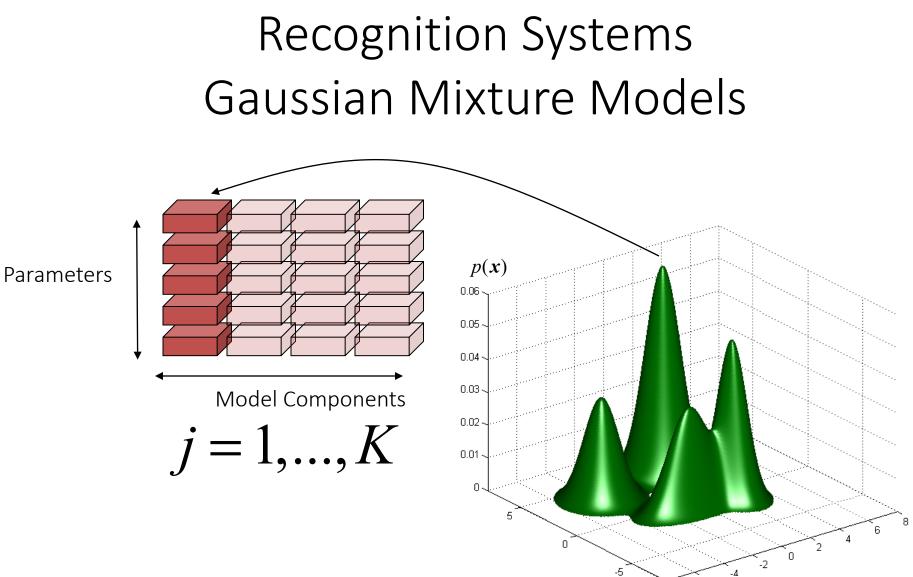
- A Gaussian mixture model (GMM) represents as the weighted sum of multiple Gaussian distributions
- Each Gaussian state i has a
 - -Mean μ_j
 - Covariance
 - Weight

$$w_{j} \equiv p(\mu = \mu_{j})$$

 \sum







Dim 2 -8 Dim 1

A Gaussian mixture model (GMM)

represents as the weighted sum of

Learning a Gaussian Mixture

Probability Model

multiple Gaussian distributions $p(\vec{x} = \vec{x}_i)$ $=\sum p(\vec{x}=\vec{x}_i,\vec{\mu}=\vec{\mu}_j)$ Total low of probability $= \sum_{i} p(\vec{\mu} = \vec{\mu}_{j}) p(\vec{x} = \vec{x}_{i} | \vec{\mu} = \vec{\mu}_{j}) \quad \text{Chain rule}$ $= \sum_{j} p(\vec{\mu} = \vec{\mu}_{j}) \frac{1}{\left(2\pi\right)^{p/2} \left|\Sigma_{j}\right|^{1/2}} e^{-\frac{1}{2} \left(\vec{x} - \vec{\mu}_{j}\right)^{T} \Sigma_{j}^{-1} \left(\vec{x} - \vec{\mu}_{j}\right)}$

Max Log-likelihood of Observed Data Samples

 \Box Log-likelihood of data $logp(x_1, x_2, x_3, ..., x_n) =$

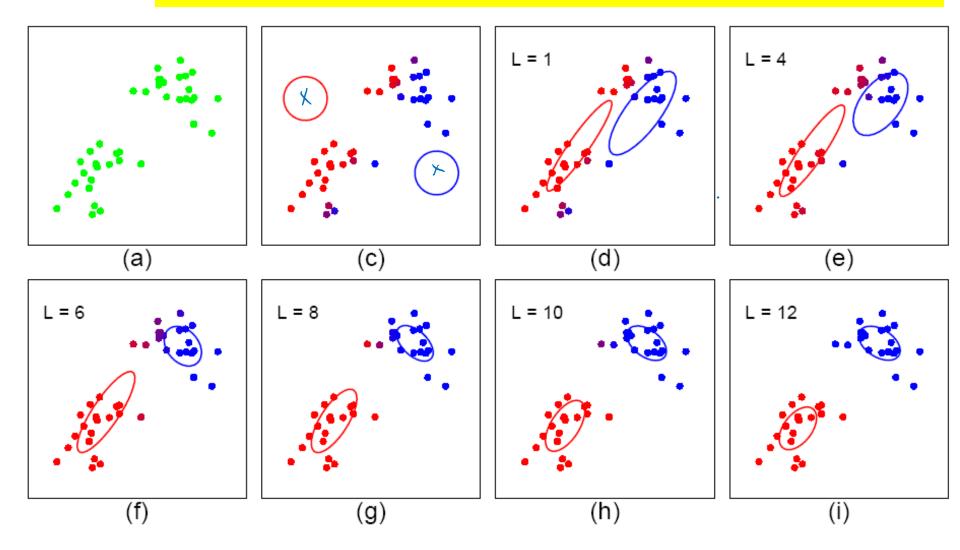
$$\log \prod_{i=1..n} \sum_{j=1..K} p(\vec{\mu} = \vec{\mu}_j) \frac{1}{\left(2\pi\right)^{p/2} \left|\Sigma_j\right|^{1/2}} e^{-\frac{1}{2} \left(\vec{x}_i - \vec{\mu}_j\right)^T \Sigma_j^{-1} \left(\vec{x}_i - \vec{\mu}_j\right)}$$

Apply MLE to find $\left\{ \{ p(\vec{\mu} = \mu_j) \}, j = 1...K \right\}$ optimal Gaussian parameters $\{ \vec{\mu}_j, \Sigma_j, j = 1...K \}$

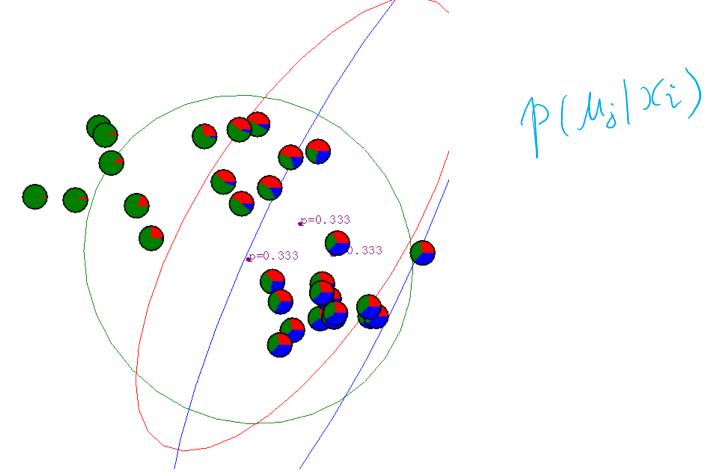
Expectation-Maximization for training GMM

- Start:
 - "Guess" the centroid and covariance for each of the K clusters
 - "Guess" the proportion of clusters, e.g., uniform prob 1/K
- Loop
 - For each point, revising its proportions belonging to each of the K clusters
 - For each cluster, revising both the mean (centroid position) and covariance (shape)

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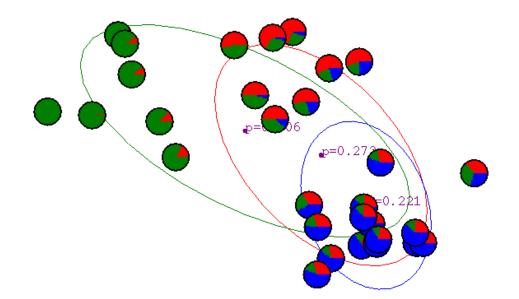


Another Gaussian Mixture Example: Start



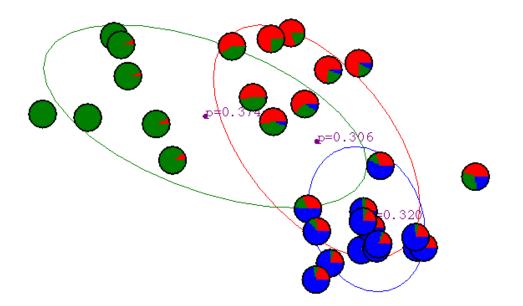
Another GMM Example: After First Iteration

For each point, revising its proportions belonging to each of the K clusters



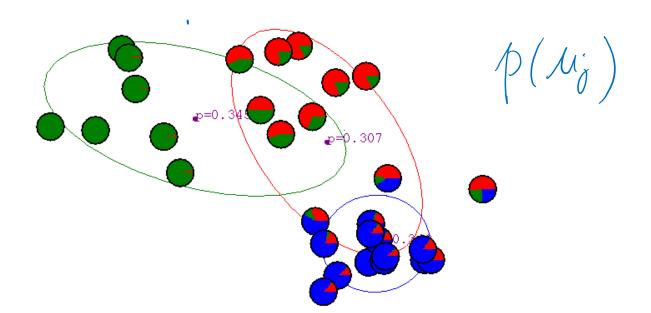
Another GMM Example: After 2nd Iteration

For each point, revising its proportions belonging to each of the K clusters



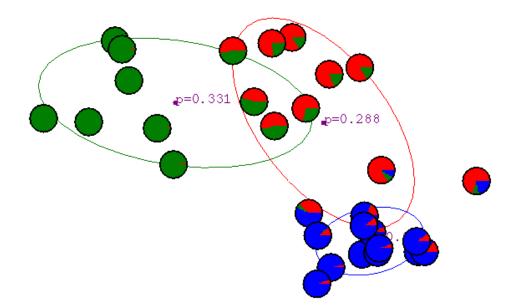
After 3rd Iteration

For each point, revising its proportions belonging to each of the K clusters



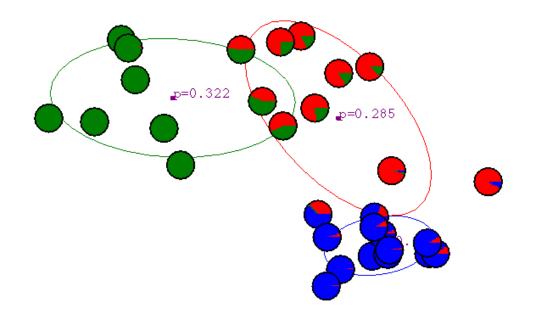
After 4th Iteration

For each point, revising its proportions belonging to each of the K clusters



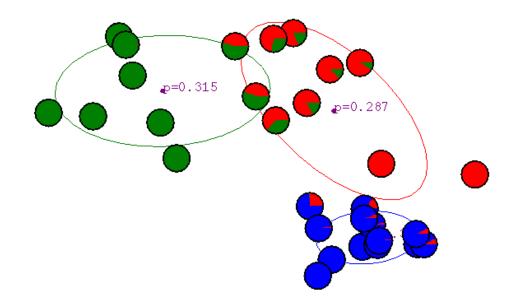
After 5th Iteration

For each point, revising its proportions belonging to each of the K clusters



After 6th Iteration

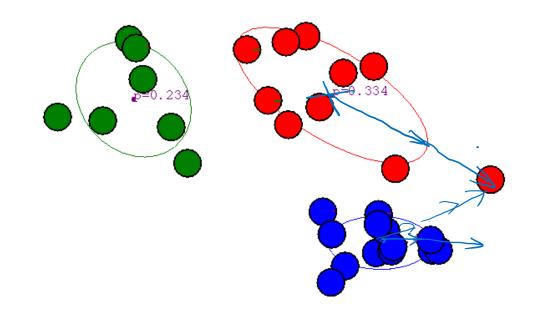
For each point, revising its proportions belonging to each of the K clusters



For each cluster, revising its mean (centroid position), covariance (shape) and proportion in the mixture

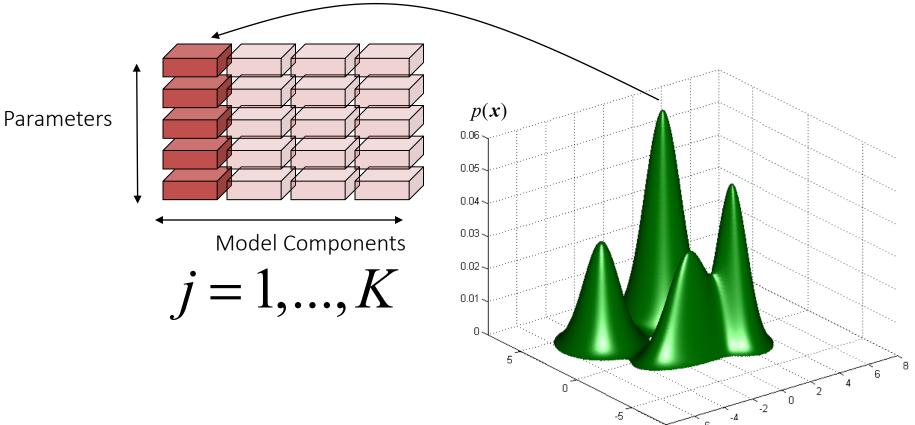
Another GMM Example: After 20th Iteration

For each point, revising its proportions belonging to each of the K clusters



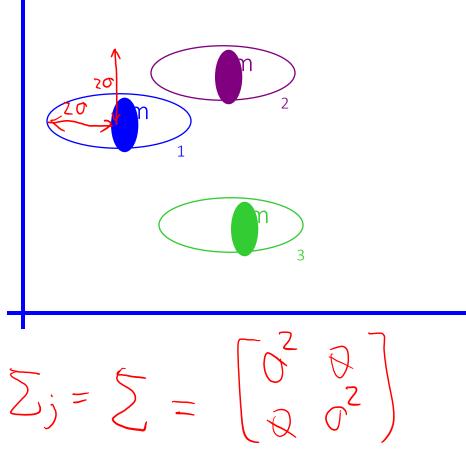
For each cluster, revising its mean (centroid position), covariance (shape) and proportion in the mixture

Recap: Gaussian Mixture Models



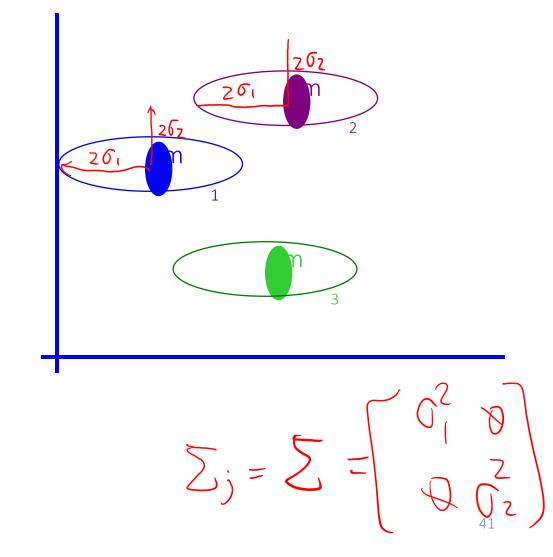
The Simplest GMM assumption

- Each component generates data from a Gaussian with
 - mean μ_i
 - Shared diagonal covariance matrix σ²



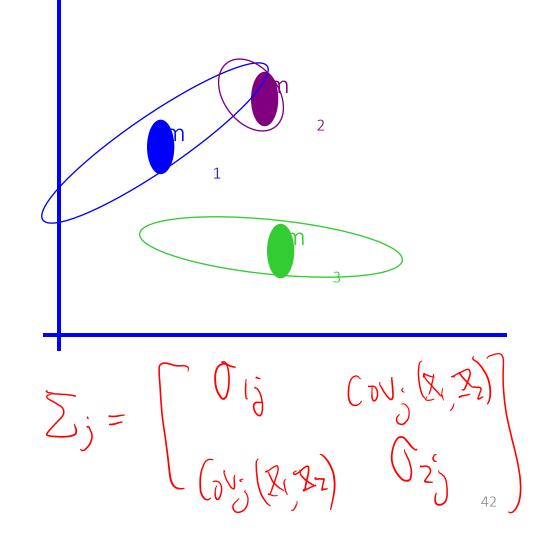
Another Simple GMM assumption

- Each component generates data from a Gaussian with
 - mean μ_i
 - Shared covariance matrix as diagonal matrix



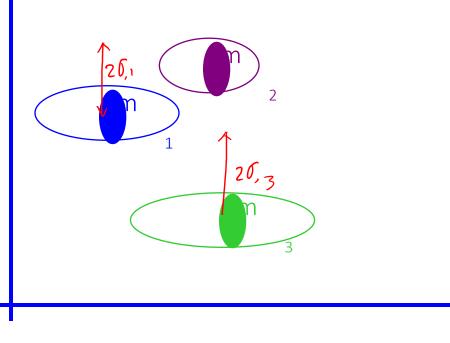
The General GMM assumption

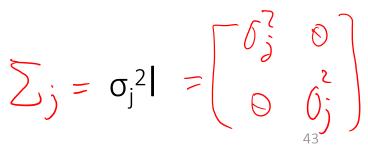
- Each component generates data from a Gaussian with
 - mean μ_i
 - covariance matrix Σ_i



Another Simple GMM assumption

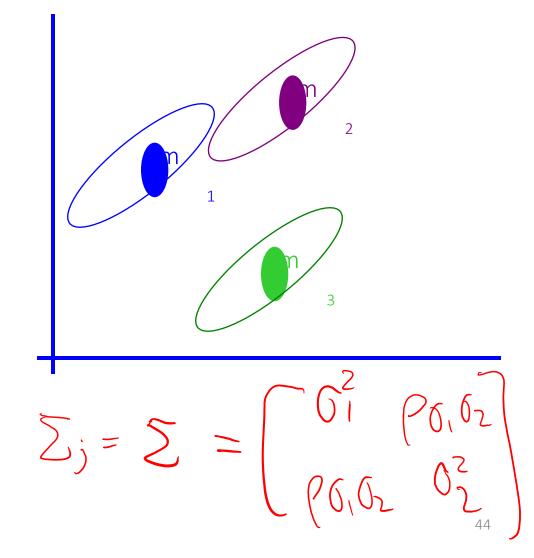
- Each component generates data from a Gaussian with
 - mean μ_i
 - Cluster-specific diagonal covariance matrix as σ_j²l





A bit More General GMM assumption

- Each component generates data from a Gaussian with
 - mean μ_i
 - Shared covariance matrix as full matrix



Concrete Equations for Learning a Gaussian Mixture

when assuming with known shared covariance

$$p(\vec{x} = \vec{x}_{i})$$

$$= \sum_{\mu_{j}} p(\vec{x} = \vec{x}_{i}, \vec{\mu} = \vec{\mu}_{j})$$

$$= \sum_{j} p(\vec{\mu} = \vec{\mu}_{j}) p(\vec{x} = \vec{x}_{i} | \vec{\mu} = \vec{\mu}_{j})$$

$$= \sum_{j} p(\vec{\mu} = \vec{\mu}_{j}) \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2} (\vec{x}_{i} - \vec{\mu}_{j})^{T} \Sigma^{-1} (\vec{x}_{i} - \vec{\mu}_{j})}$$
Assuming Known and Shared

E-step (vs. Assignment Step in K-means)

when assuming with known shared covariance

$$\begin{split} & \underset{E-\text{Step}}{\text{Hij}} = \begin{cases} 0\\ 1\\ E_{ij} \end{bmatrix} = p(\mu = \mu_{j} \mid x = x_{i}) \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\text{E[}z_{ij} \end{bmatrix}} = p(\mu = \mu_{j} \mid \mu = \mu_{j})p(\mu = \mu_{j}) \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} p(x = x_{i} \mid \mu = \mu_{s})p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\text{How} \ x_{i} \ belongs} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\text{How} \ x_{i} \ belongs} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} p(x = x_{i} \mid \mu = \mu_{s})p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\text{How} \ x_{i} \ belongs} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} p(x = x_{i} \mid \mu = \mu_{s})p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\frac{1}{2\pi}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{j})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})^{T} \Sigma^{-1}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s})} \\ & \underset{P(M = M_{j} \mid x = x_{i})}{\sum_{s=1}^{k} \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_{s})} p(\mu = \mu_{s}$$

Learning a Gaussian Mixture

when assuming with known shared covariance

M-Step

$$\mu_{j}^{(\ddagger, l)} \leftarrow \frac{1}{\sum_{i=1}^{n} E[z_{ij}]} \sum_{i=1}^{n} E[z_{ij}] x_{i}$$

$$\sum_{i=1}^{n} E[z_{ij}]^{i=1}$$

$$p(\mu = \mu_{j}) \leftarrow \frac{1}{n} \sum_{i=1}^{n} E[z_{ij}]$$

Covariance: \sum_{j} (j: 1 to K) can also be derived in the M-step under a full setting

M-step (vs. Centroid Step in K-means)

when assuming with known shared covariance

M-Step

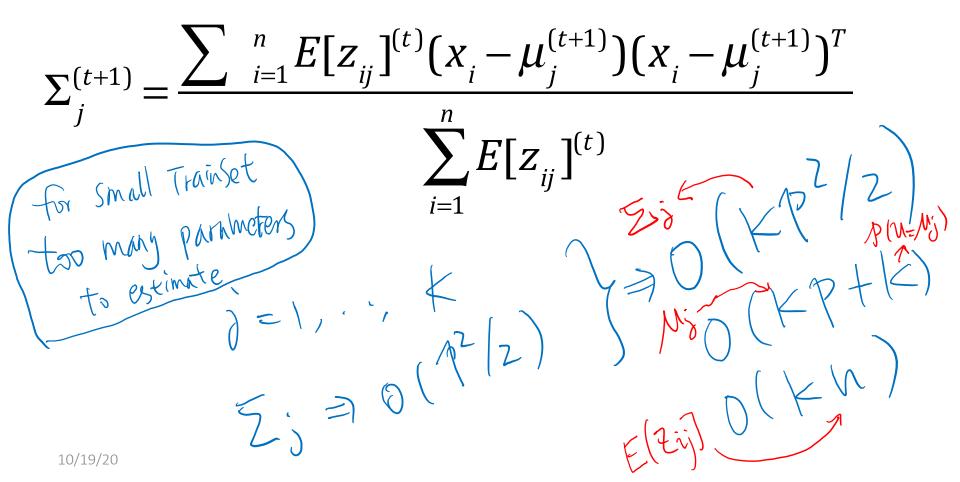
$$(t_{i}) = (entroid = N_{i} \sum_{j=1}^{n} K_{i})$$

$$\mu_{j} \leftarrow \frac{1}{n} \sum_{i=1}^{n} E[z_{ij}]^{i} = (t_{i})$$

$$p(\mu = \mu_{j}) \leftarrow \frac{1}{n} \sum_{i=1}^{n} E[z_{ij}]^{i} = (t_{i})$$

Covariance: \sum_{j} (j: 1 to K) will also be derived in the M-step under a full setting

M-step for Estimating Dr. Yanjun Qi / UVA CS unknown Covariance Matrix (more general, details in EM-Extra lecture)



Recap: Expectation-Maximization for training GMM

- Start:
 - "Guess" the centroid and covariance for each of the K clusters
 - "Guess" the proportion of clusters, e.g., uniform prob 1/K
- Loop
 - For each point, revising its proportions belonging to each of the K clusters
 - For each cluster, revising both the mean (centroid position) and covariance (shape)

Partitional : Gaussian Mixture Model

- 1. Review of Gaussian Distribution
- 2. GMM for clustering : basic algorithm
- 3. GMM connecting to K-means
- 4. Problems of GMM and K-means

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Recap: K-means iterative learning

$$\arg\min_{\{\vec{C}_{j}, m_{i,j}\}} \sum_{j=1}^{K} \sum_{i=1}^{n} m_{i,j} \left(\vec{x}_{i} - \vec{C}_{j}\right)^{2}$$

Memberships
$$\{m_{i,j}\}$$
 and centers $\{C_j\}$ are correlated.
E-Step Given centers $\{\vec{C}_j\}, m_{i,j} = \begin{cases} 1 & j = \arg\min(\vec{x}_i - \vec{C}_j)^2 \\ 0 & \text{otherwise} \end{cases}$
M-Step Given memberships $\{m_{i,j}\}, \vec{C}_j = \frac{\sum_{i=1}^n m_{i,j} \vec{x}_i}{\sum_{i=1}^n m_{i,j}}$

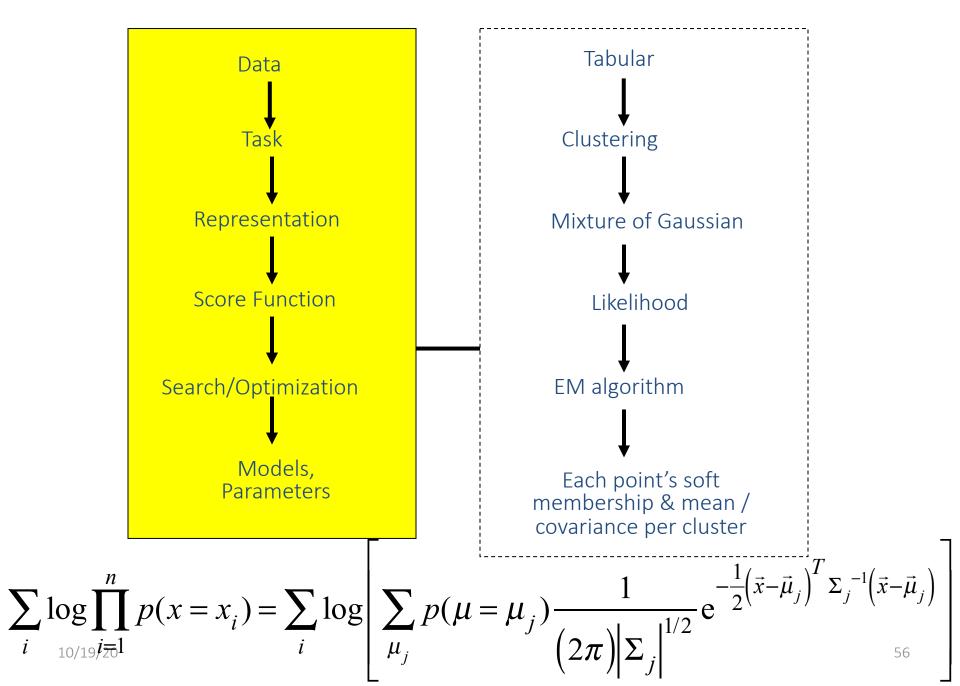
Compare: K-means

- The EM algorithm for mixtures of Gaussians is like a "soft version" of the K-means algorithm.
- In the K-means "E-step" we do hard assignment:
- In the K-means "M-step" we update the means as the weighted sum of the data, but now the weights are 0 or 1:

$$\bigcup_{i} \mathcal{M} : \sum_{i} \log \prod_{i=1}^{n} p(x=x_{i}) = \sum_{i} \log \left[\sum_{\mu_{j}}^{\mathfrak{d}=1, \cdot, \mathbf{k}} \sum_{\mu_{j}} p(\mu=\mu_{j}) \frac{1}{(2\pi) |\Sigma|^{1/2}} e^{-\frac{1}{2} (\vec{x}-\vec{\mu}_{j})^{T} \Sigma^{-1} (\vec{x}-\vec{\mu}_{j})} \right]$$

- K-Mean only detect spherical clusters.
- GMM can adjust its self to elliptic shape clusters.

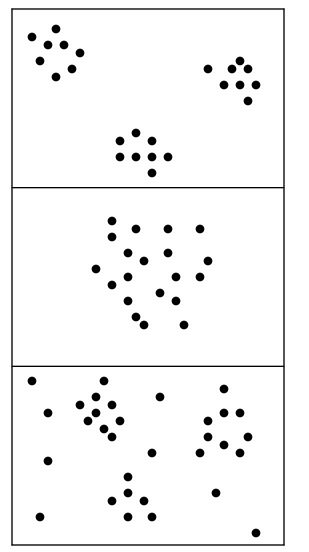




Partitional : Gaussian Mixture Model

- 1. Review of Gaussian Distribution
- 2. GMM for clustering : basic algorithm
- 3. GMM connecting to K-means
- 4. Problems of GMM and K-means

Unsupervised Learning: not as hard as it looks



Sometimes easy

Sometimes impossible

and sometimes in between

Dr. Yanjun Qi / UVA CS

Problems (I)

- Both k-means and mixture models need to compute centers of clusters and explicit distance measurement
 - Given strange distance measurement, the center of clusters can be hard to compute

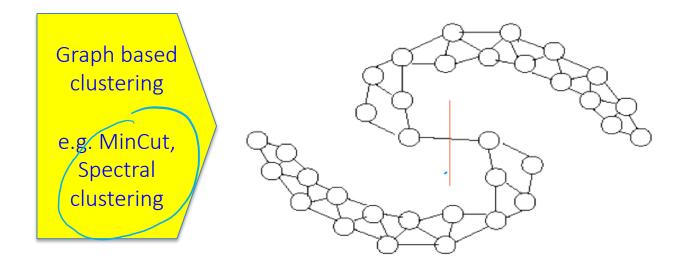
E.g.,
$$\|\vec{x} - \vec{x}'\|_{\infty} = \max\left(\|x_1 - x_1'\|, |x_2 - x_2'|, \dots, |x_p - x_p'|\right)$$

$$\begin{array}{c} \times & \vee \\ \bullet & \bullet \\ & \bullet & \bullet \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

tight

Problem (II)

- Both k-means and mixture models look for compact clustering structures
 - In some cases, connected clustering structures are more desirable



e.g. Image Segmentation through minCut



(a)



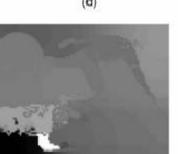
(b)



(c)



(d)



10/19/20



(e)





(f)



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References

- Hastie, Trevor, et al. The elements of statistical learning. Vol. 2. No. 1. New York: Springer, 2009.
- □ Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Big thanks to Prof. Ziv Bar-Joseph @ CMU for allowing me to reuse some of his slides
- □ clustering slides from Prof. Rong Jin @ MSU