Clustering

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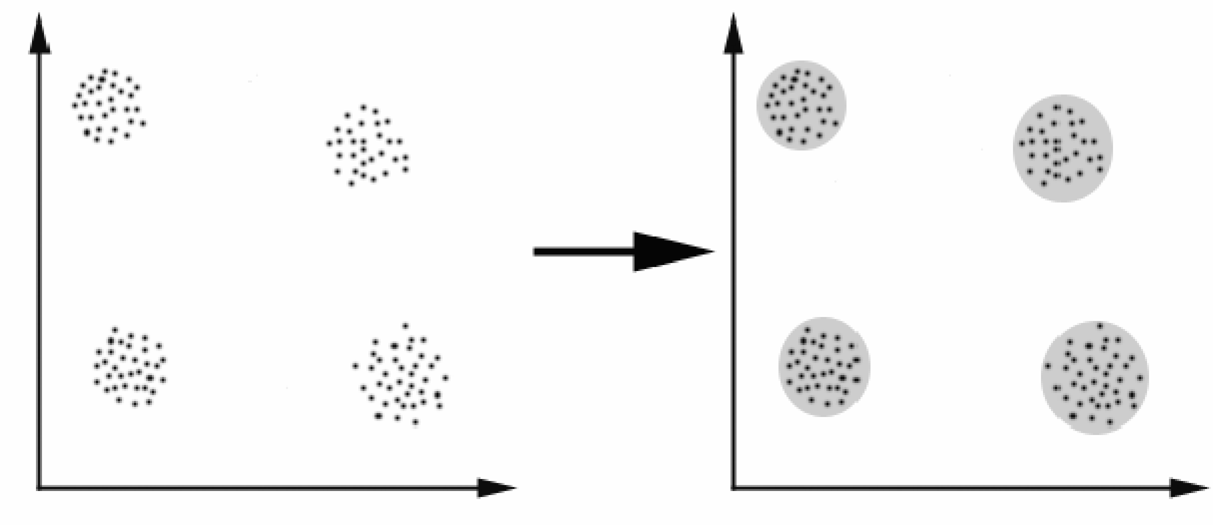
Outline

- Flat clustering
  - Mixture of Gaussians
  - K-means
- Hierarchical clustering
  - bottom-up
- Spectral based clustering
- Applications

Clustering

- Given set of data points, group them
- Unsupervised learning
- Learn the similarity. Which patient are similar? (or customers, faces, earthquakes, …)

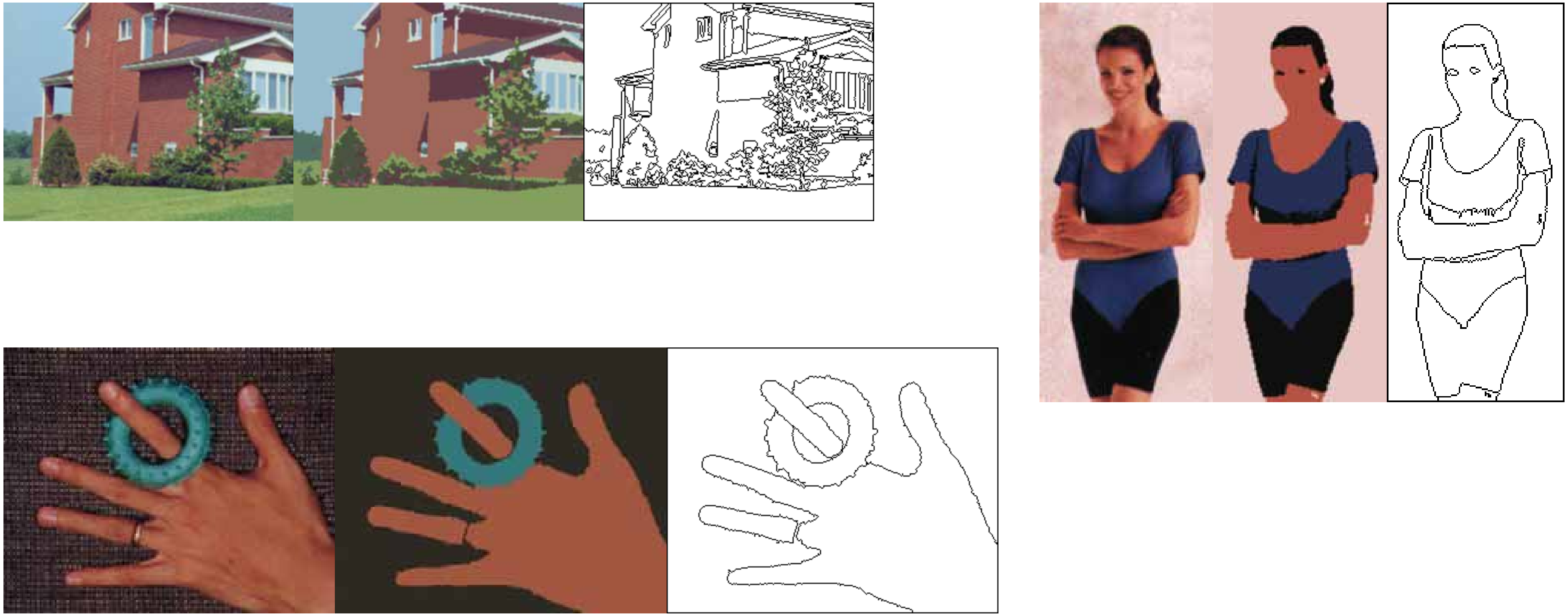


Clustering vs. Classification

- **Clustering**
  - **Instance:** $\{\mathbf{x}_i\}_{i=1}^N$
  - **Learn:** $<\mathbf{x}_i, t_i>$ and/or mapping from $\mathbf{x}$ to $t(\mathbf{x})$

- **Classification/Regression**
  - **Instance:** $<\mathbf{x}_i, t_i>$
  - **Learn:** mapping from $\mathbf{x}$ to $t(\mathbf{x})$

Clustering: image segmentation



Mean-shift segmentation

Mixtures of Gaussians

- Mixture distribution:
  - Assume *P(x)* is a mixture of K different Gaussians
  - Assume each data point, x, is generated by 2-step process
    - Choose one of the K Gaussians as label z
    - Generate x according to the Gaussian $N(\mu_z, \Sigma_z)$

$$P(\mathbf{x}) = \sum_{z=1}^{K} P(Z = z \mid \pi) N(\mathbf{x} \mid \mu_z, \Sigma_z)$$

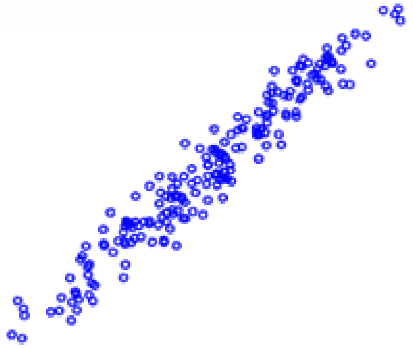
- What object function shall we optimize?
  - Maximize data likelihood

Mixtures of Gaussians (cont.)

- Multivariate Gaussian model

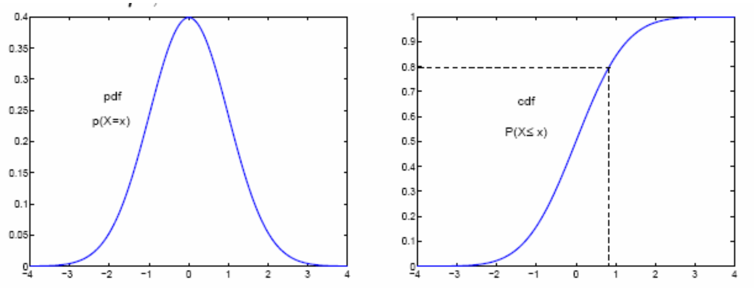
$$p(\mathbf{x}|\mu,\Sigma) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\{ -\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu) \}$$

- How to generate it?

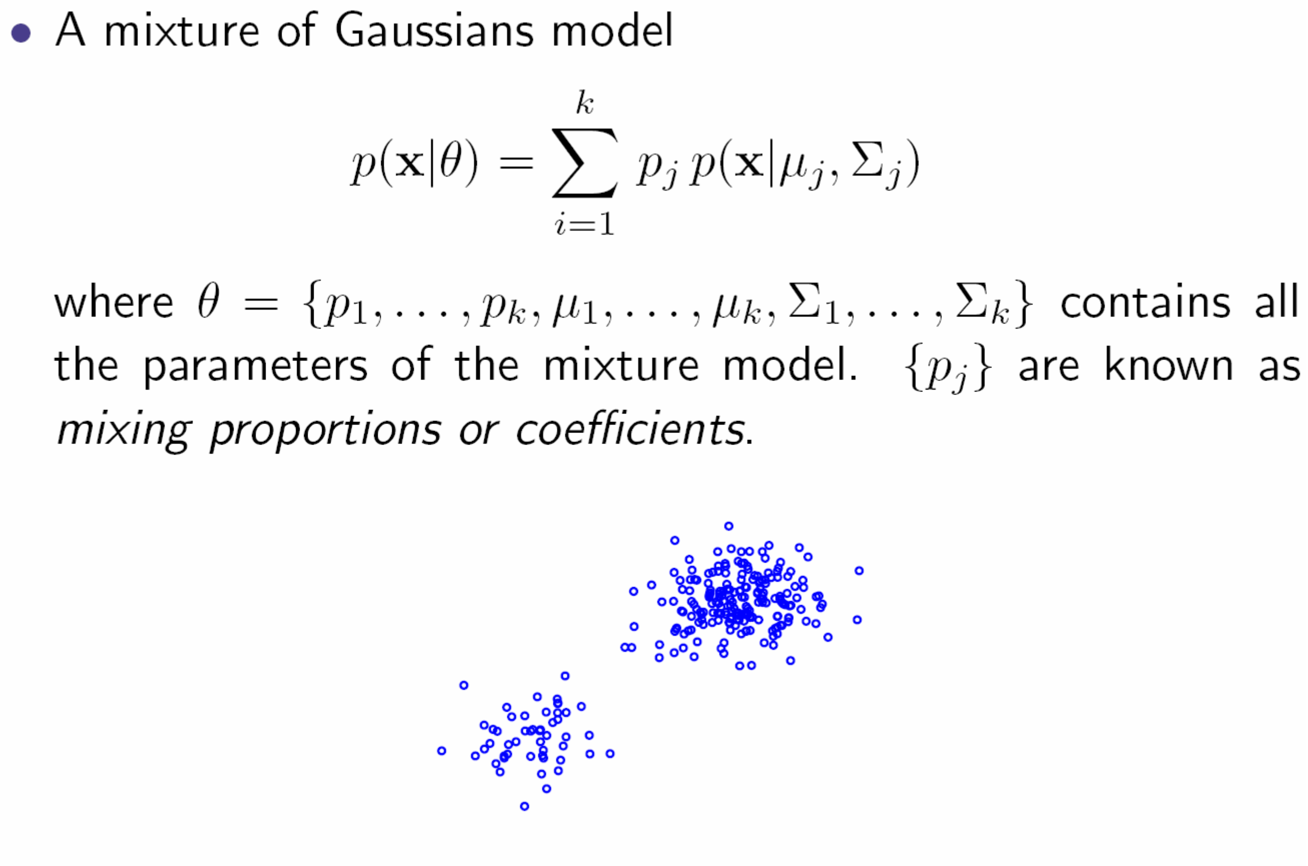


$$\begin{aligned} F_{\mu,\sigma^2}(x) &= \int_{-\infty}^{x} p(z|\mu,\sigma^2)dz \\ u \sim \text{Uniform}(0,1) &\Rightarrow x = F^{-1}_{\mu,\sigma^2}(u) \sim p(x|\mu,\sigma^2) \end{aligned}$$

$$\begin{aligned} z_i &\sim p(z_i|\mu=0,\sigma^2=1), \quad \mathbf{z} = [z_1,\dots,z_d]^T \\ \mathbf{x} &= \Sigma^{1/2}\mathbf{z} + \mu \end{aligned}$$



Multi-variate density estimation



- A mixture of Gaussians model

$$p(\mathbf{x}|\theta) = \sum_{i=1}^{k} p_j \, p(\mathbf{x}|\mu_j, \Sigma_j)$$

where $\theta = \{p_1, \ldots, p_k, \mu_1, \ldots, \mu_k, \Sigma_1, \ldots, \Sigma_k\}$ contains all the parameters of the mixture model. $\{p_j\}$ are known as *mixing proportions or coefficients*.

Mixtures of Gaussians: Wishart distribution

- A mixture of Gaussian Model:

$$p(\mathbf{x}|\theta) = \sum_{i=1}^{k} p_j \, p(\mathbf{x}|\mu_j, \Sigma_j)$$

High dimensional parameters

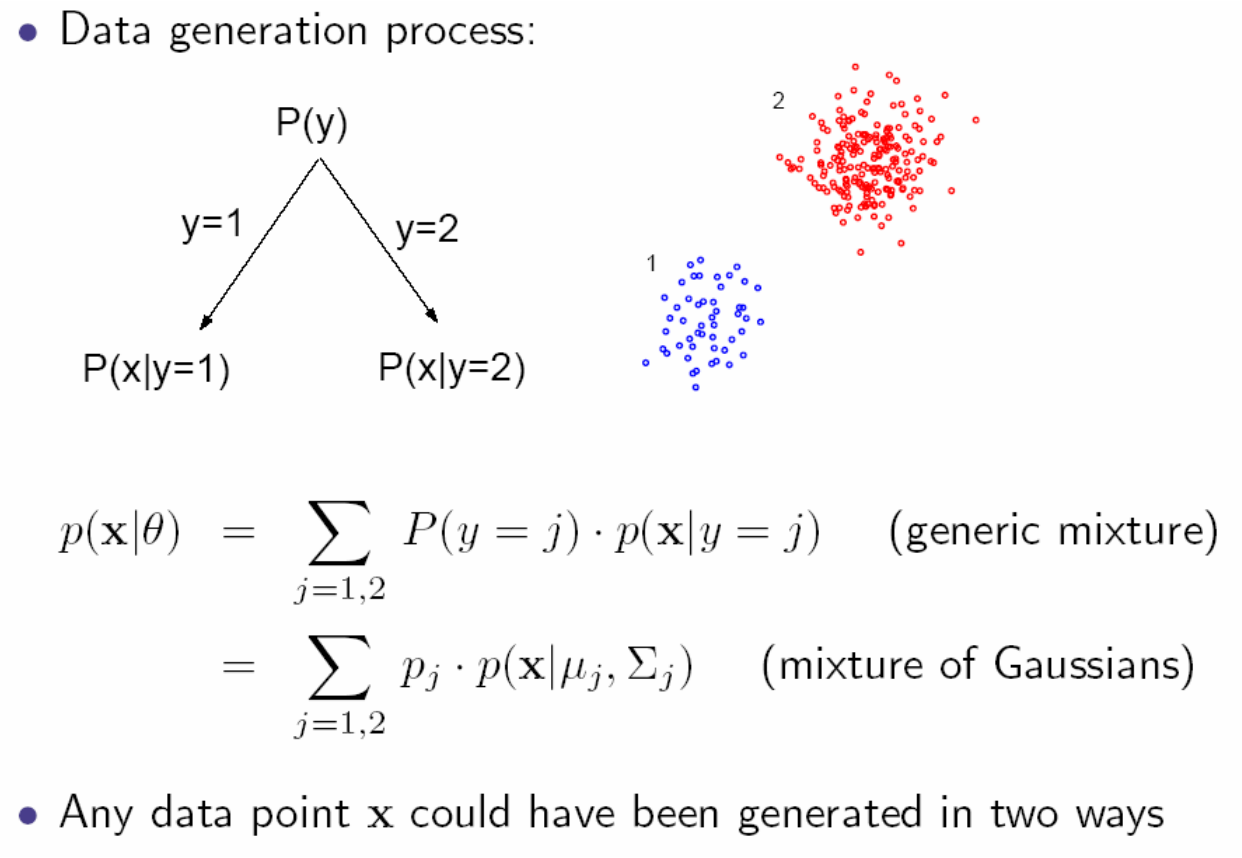
$$\theta = \{p_1, \ldots, p_k, \mu_1, \ldots, \mu_k, \underline{\Sigma_1, \ldots, \Sigma_k}\}$$

- Wishart prior

$$P(\Sigma|S, n') \propto \frac{1}{|\Sigma|^{n'/2}} \exp\left(-\frac{n'}{2}\text{Trace}(\Sigma^{-1}S)\right)$$

$$\begin{aligned} S &= \text{“prior” covariance matrix} \\ n' &= \text{equivalent sample size} \end{aligned}$$

Mixture density



- Data generation process:

$$p(\mathbf{x}|\theta) = \sum_{j=1,2} P(y=j)\cdot p(\mathbf{x}|y=j) \quad \text{(generic mixture)}$$

$$= \sum_{j=1,2} p_j \cdot p(\mathbf{x}|\mu_j, \Sigma_j) \quad \text{(mixture of Gaussians)}$$

- Any data point $\mathbf{x}$ could have been generated in two ways

Mixture density

- If we are given just $\mathbf{x}$ we don't know which mixture component this example came from

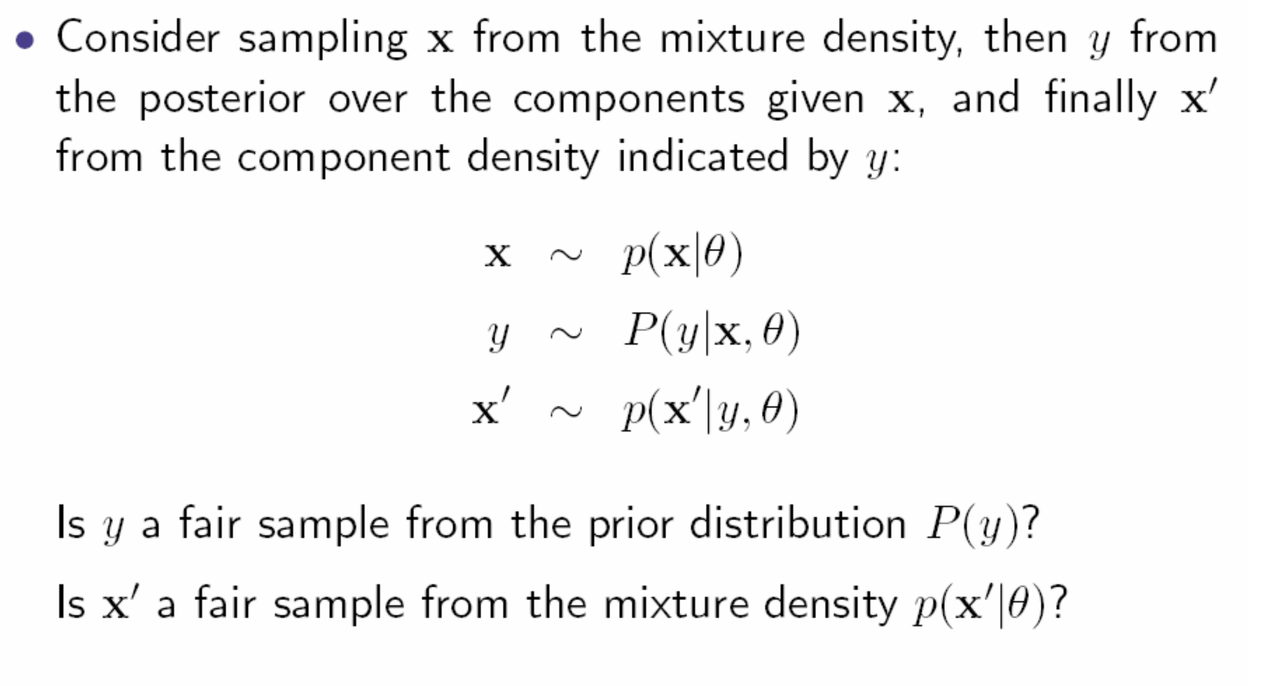
$$p(\mathbf{x}|\theta) \;=\; \sum_{j=1,2} p_j p(\mathbf{x}|\mu_j, \Sigma_j)$$

- We can evaluate the posterior probability that an observed $\mathbf{x}$ was generated from the first mixture component

$$\begin{aligned} P(y=1|\mathbf{x},\theta) &= \frac{P(y=1)\cdot p(\mathbf{x}|y=1)}{\sum_{j=1,2} P(y=j)\cdot p(\mathbf{x}|y=j)} \\ &= \frac{p_1\, p(\mathbf{x}|\mu_1,\Sigma_1)}{\sum_{j=1,2} p_j\, p(\mathbf{x}|\mu_j,\Sigma_j)} \end{aligned}$$

- This solves a *credit assignment* problem

Mixture density: posterior sampling



- Consider sampling $\mathbf{x}$ from the mixture density, then y from the posterior over the components given $\mathbf{x}$, and finally $\mathbf{x}'$ from the component density indicated by y:

$$\begin{aligned} \mathbf{x} &\sim p(\mathbf{x}|\theta) \\ y &\sim P(y|\mathbf{x},\theta) \\ \mathbf{x}' &\sim p(\mathbf{x}'|y,\theta) \end{aligned}$$

Is y a fair sample from the prior distribution $P(y)$?

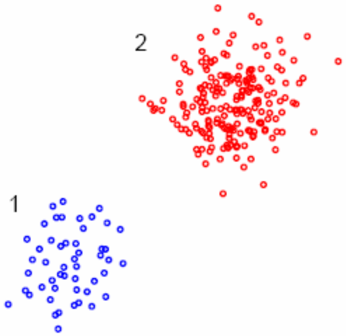
Is $\mathbf{x}'$ a fair sample from the mixture density $p(\mathbf{x}'|\theta)$?

Mixture density estimation

- Suppose we want to estimate a two component mixture of Gaussians model.

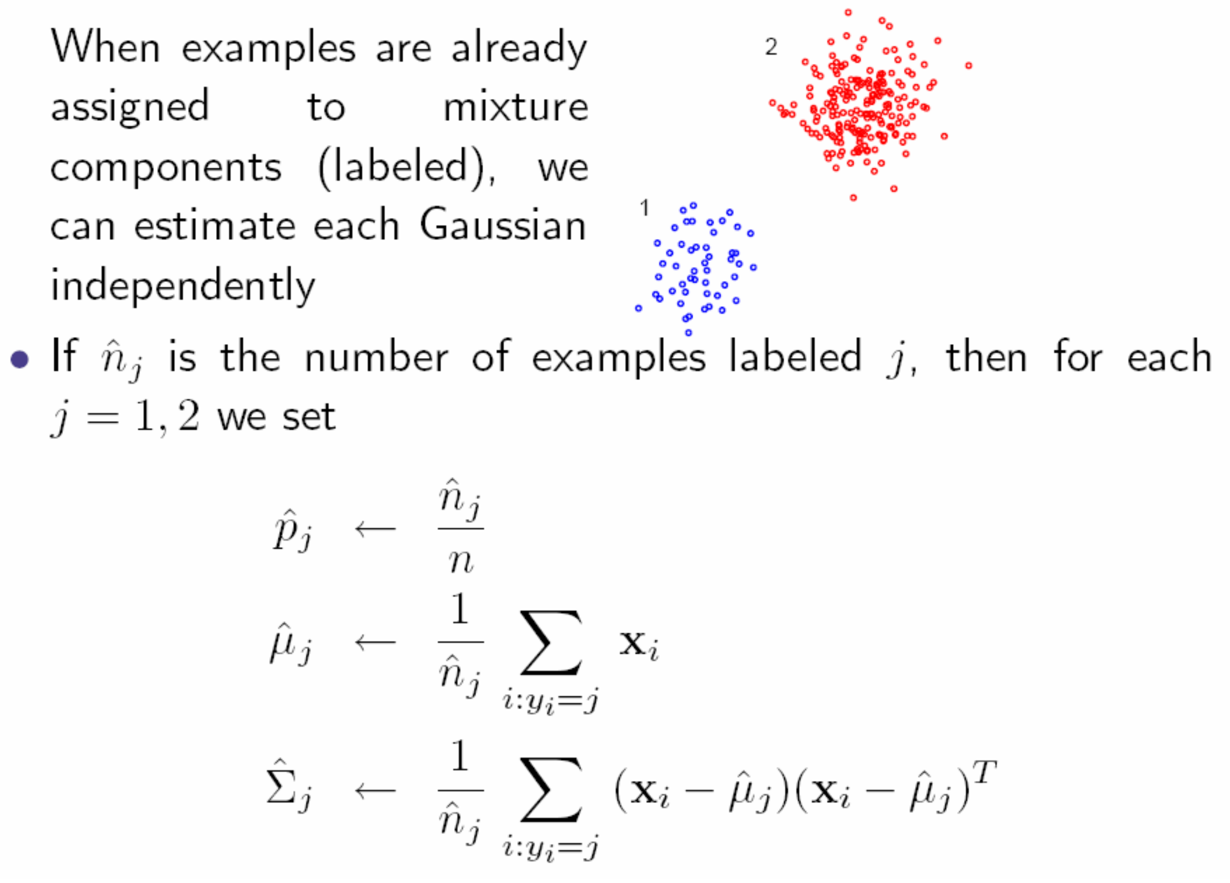
$$p(\mathbf{x}|\theta) = p_1\, p(\mathbf{x}|\mu_1, \Sigma_1) + p_2\, p(\mathbf{x}|\mu_2, \Sigma_2)$$

- If each example $\mathbf{x}_i$ in the training set were labeled $y_i = 1, 2$ according to which mixture component $(1$ or $2)$ had generated it, then the estimation would be easy.



- Labeled examples $\Rightarrow$ no credit assignment problem

Mixture density estimation

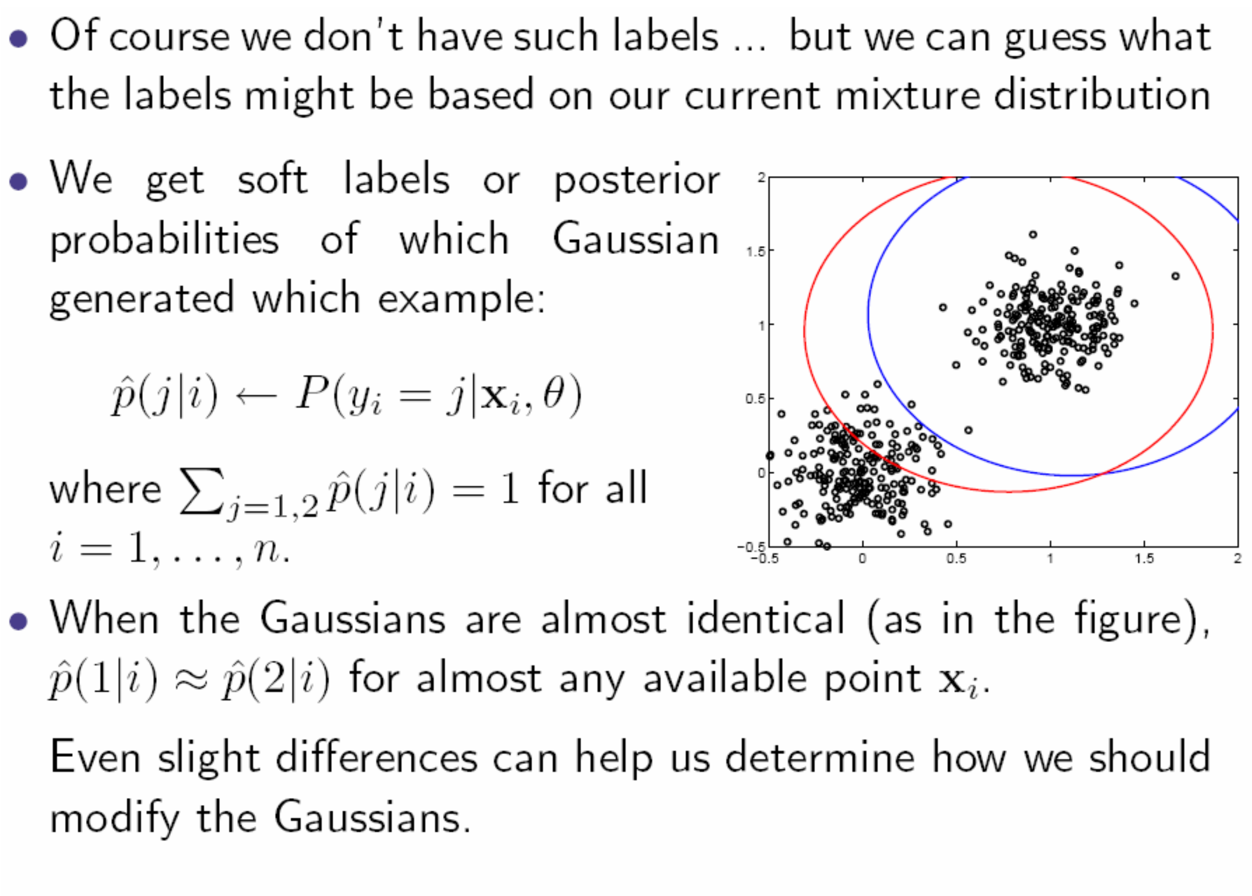


When examples are already assigned to mixture components (labeled), we can estimate each Gaussian independently

- If $\hat{n}_j$ is the number of examples labeled j, then for each $j = 1, 2$ we set

$$\begin{aligned}
\hat{p}_j &\leftarrow \frac{\hat{n}_j}{n} \\
\hat{\mu}_j &\leftarrow \frac{1}{\hat{n}_j} \sum_{i:y_i=j} \mathbf{x}_i \\
\hat{\Sigma}_j &\leftarrow \frac{1}{\hat{n}_j} \sum_{i:y_i=j} (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T
\end{aligned}$$

Mixture density estimation: credit assignment



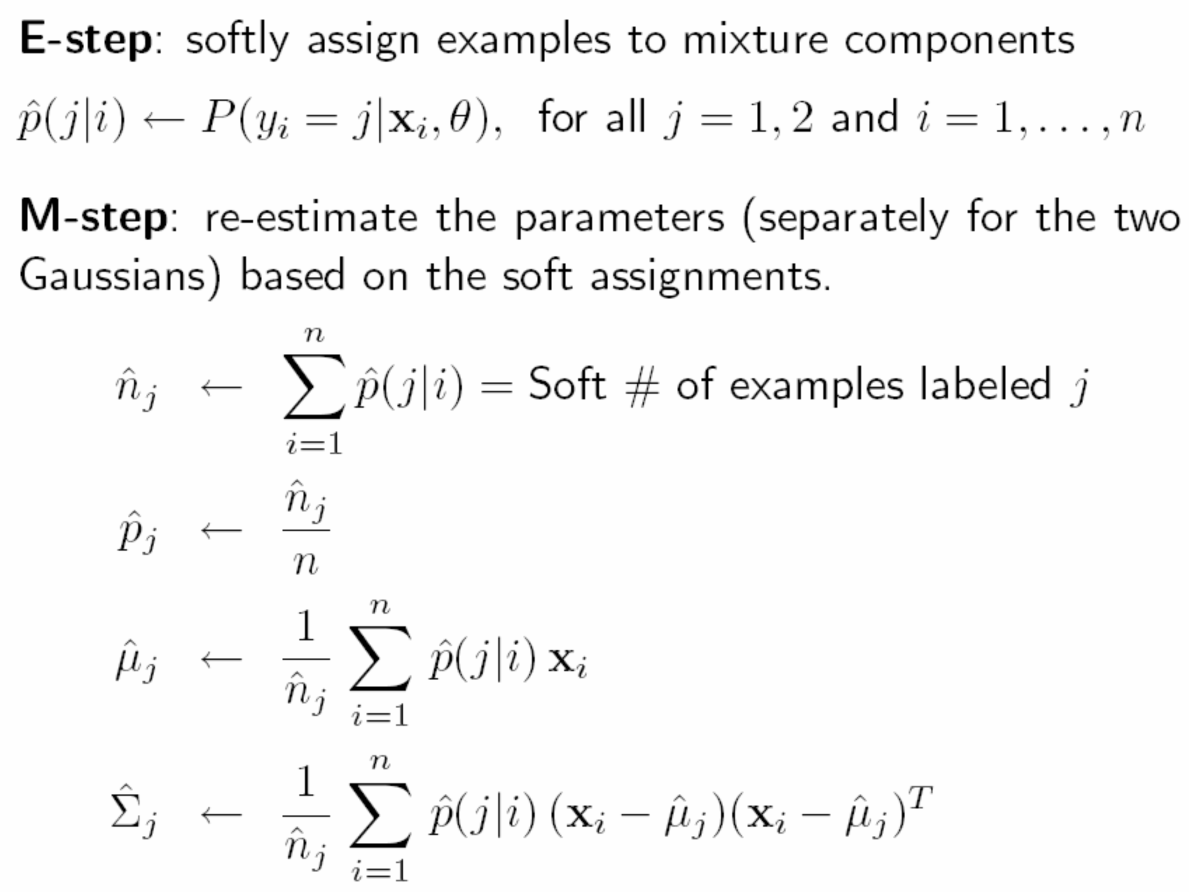
- Of course we don't have such labels ... but we can guess what the labels might be based on our current mixture distribution
- We get soft labels or posterior probabilities of which Gaussian generated which example:

  $$\hat{p}(j|i) \leftarrow P(y_i = j|\mathbf{x}_i, \theta)$$

  where $\sum_{j=1,2} \hat{p}(j|i) = 1$ for all $i = 1, \ldots, n$.
- When the Gaussians are almost identical (as in the figure), $\hat{p}(1|i) \approx \hat{p}(2|i)$ for almost any available point $\mathbf{x}_i$.

  Even slight differences can help us determine how we should modify the Gaussians.

The EM algorithm



E-step: softly assign examples to mixture components

$\hat{p}(j|i) \leftarrow P(y_i = j|\mathbf{x}_i, \theta)$, for all $j = 1, 2$ and $i = 1, \ldots, n$

M-step: re-estimate the parameters (separately for the two Gaussians) based on the soft assignments.

$$\hat{n}_j \leftarrow \sum_{i=1}^{n} \hat{p}(j|i) = \text{Soft } \# \text{ of examples labeled } j$$

$$\hat{p}_j \leftarrow \frac{\hat{n}_j}{n}$$

$$\hat{\mu}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \hat{p}(j|i)\, \mathbf{x}_i$$

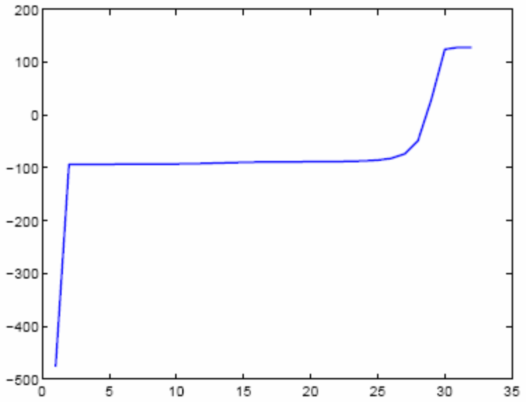
$$\hat{\Sigma}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \hat{p}(j|i)\, (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T$$

The EM-algorithm

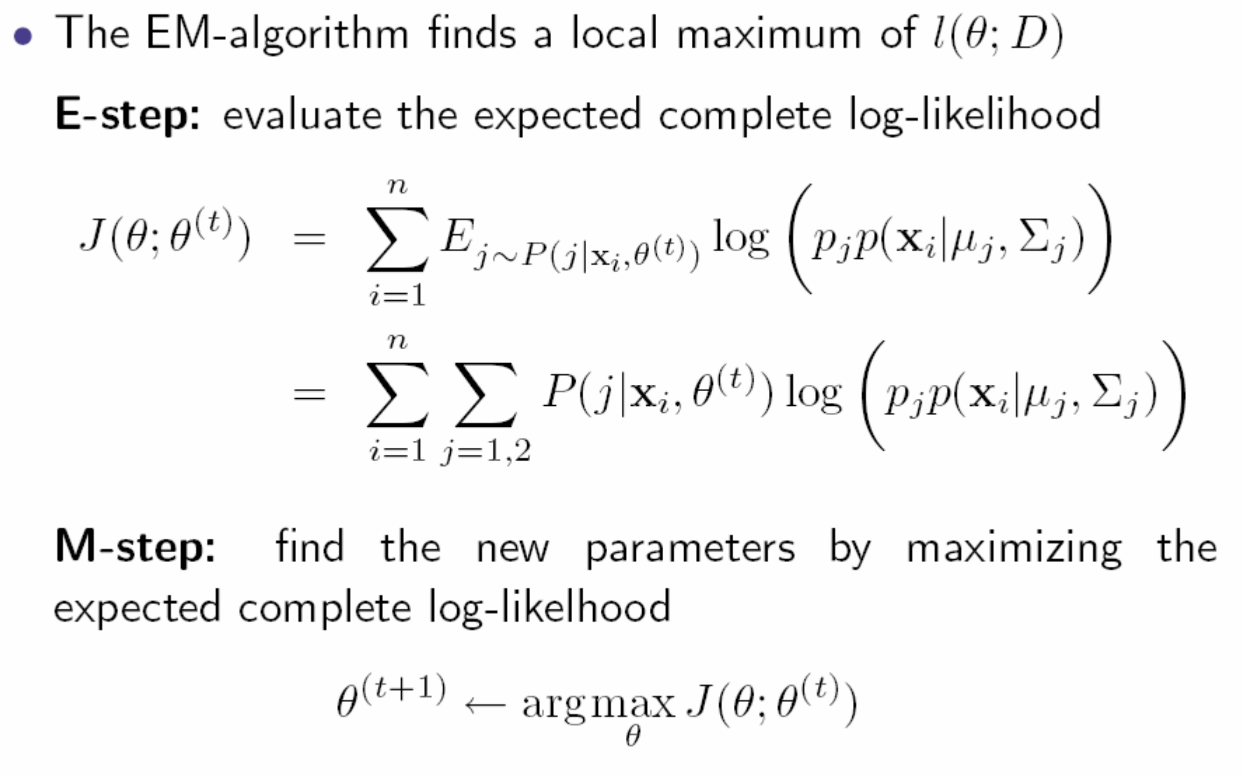
- Each iteration of the EM-algorithm *monotonically* increases the (log-)likelihood of the n training examples $\mathbf{x}_1, \ldots, \mathbf{x}_n$:

$$\log p(\text{ data } | \theta) = \sum_{i=1}^{n} \log \left(\overbrace{p_1\, p(\mathbf{x}_i | \mu_1, \Sigma_1) + p_2\, p(\mathbf{x}_i | \mu_2, \Sigma_2)}^{p(\mathbf{x}_i|\theta)} \right)$$

where $\theta = \{p_1, p_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$ contains all the parameters of the mixture model.



The EM algorithm



- The EM-algorithm finds a local maximum of $l(\theta; D)$

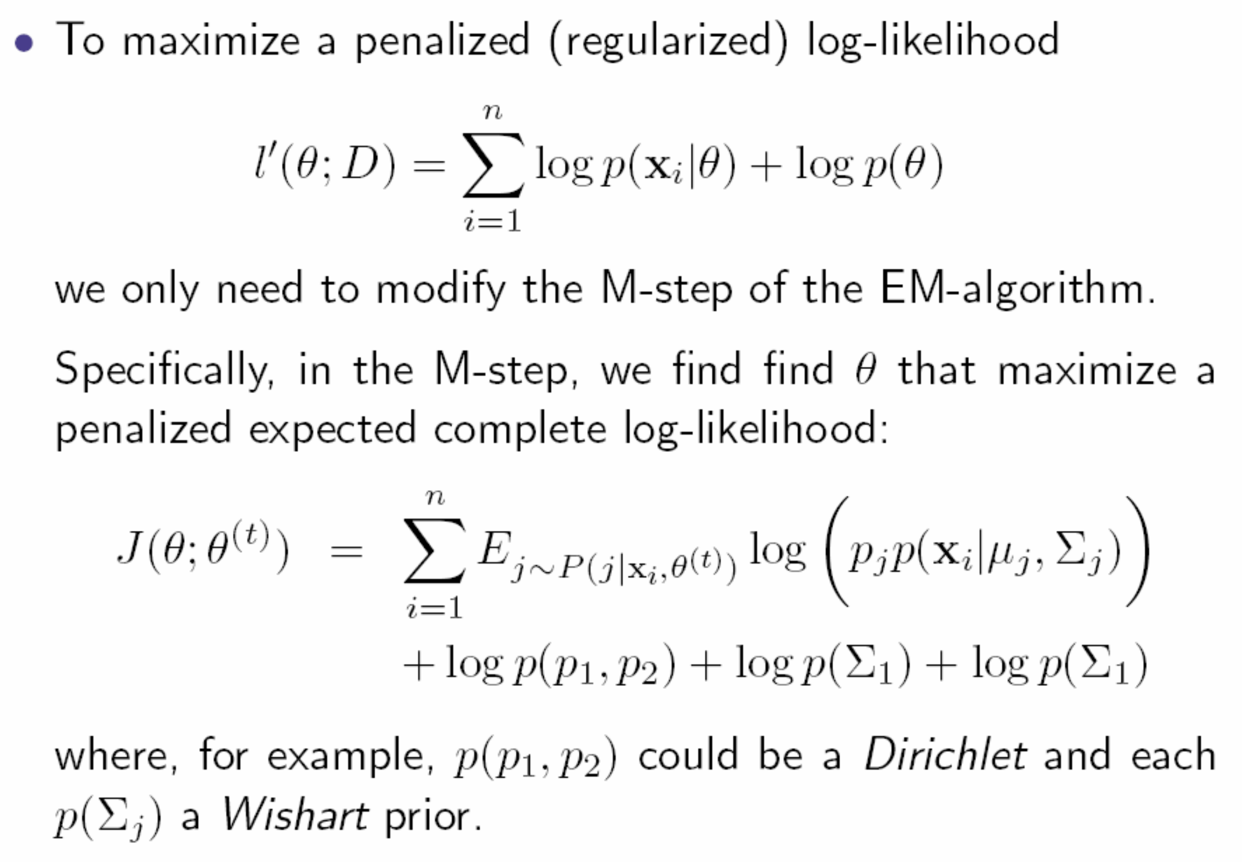
E-step: evaluate the expected complete log-likelihood

$$\begin{aligned} J(\theta; \theta^{(t)}) &= \sum_{i=1}^{n} E_{j \sim P(j|\mathbf{x}_i, \theta^{(t)})} \log \left(p_j p(\mathbf{x}_i|\mu_j, \Sigma_j) \right) \\ &= \sum_{i=1}^{n} \sum_{j=1,2} P(j|\mathbf{x}_i, \theta^{(t)}) \log \left(p_j p(\mathbf{x}_i|\mu_j, \Sigma_j) \right) \end{aligned}$$

M-step: find the new parameters by maximizing the expected complete log-likelihood

$$\theta^{(t+1)} \leftarrow \arg\max_{\theta} J(\theta; \theta^{(t)})$$

Regularized EM algorithm



- To maximize a penalized (regularized) log-likelihood

$$l'(\theta; D) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta) + \log p(\theta)$$

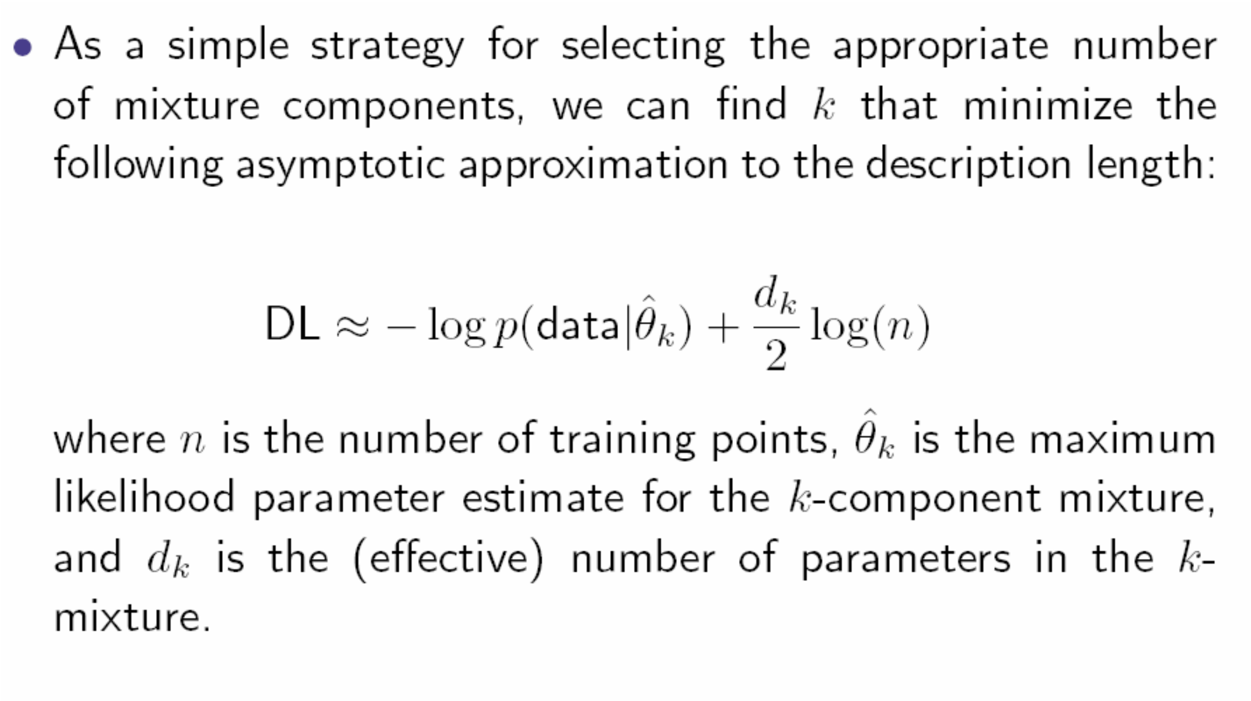
we only need to modify the M-step of the EM-algorithm.

Specifically, in the M-step, we find find θ that maximize a penalized expected complete log-likelihood:

$$\begin{aligned} J(\theta; \theta^{(t)}) &= \sum_{i=1}^{n} E_{j \sim P(j|\mathbf{x}_i, \theta^{(t)})} \log \Big(p_j p(\mathbf{x}_i|\mu_j, \Sigma_j) \Big) \\ &\quad + \log p(p_1, p_2) + \log p(\Sigma_1) + \log p(\Sigma_1) \end{aligned}$$

where, for example, $p(p_1, p_2)$ could be a *Dirichlet* and each $p(\Sigma_j)$ a *Wishart* prior.

Selecting the number of components

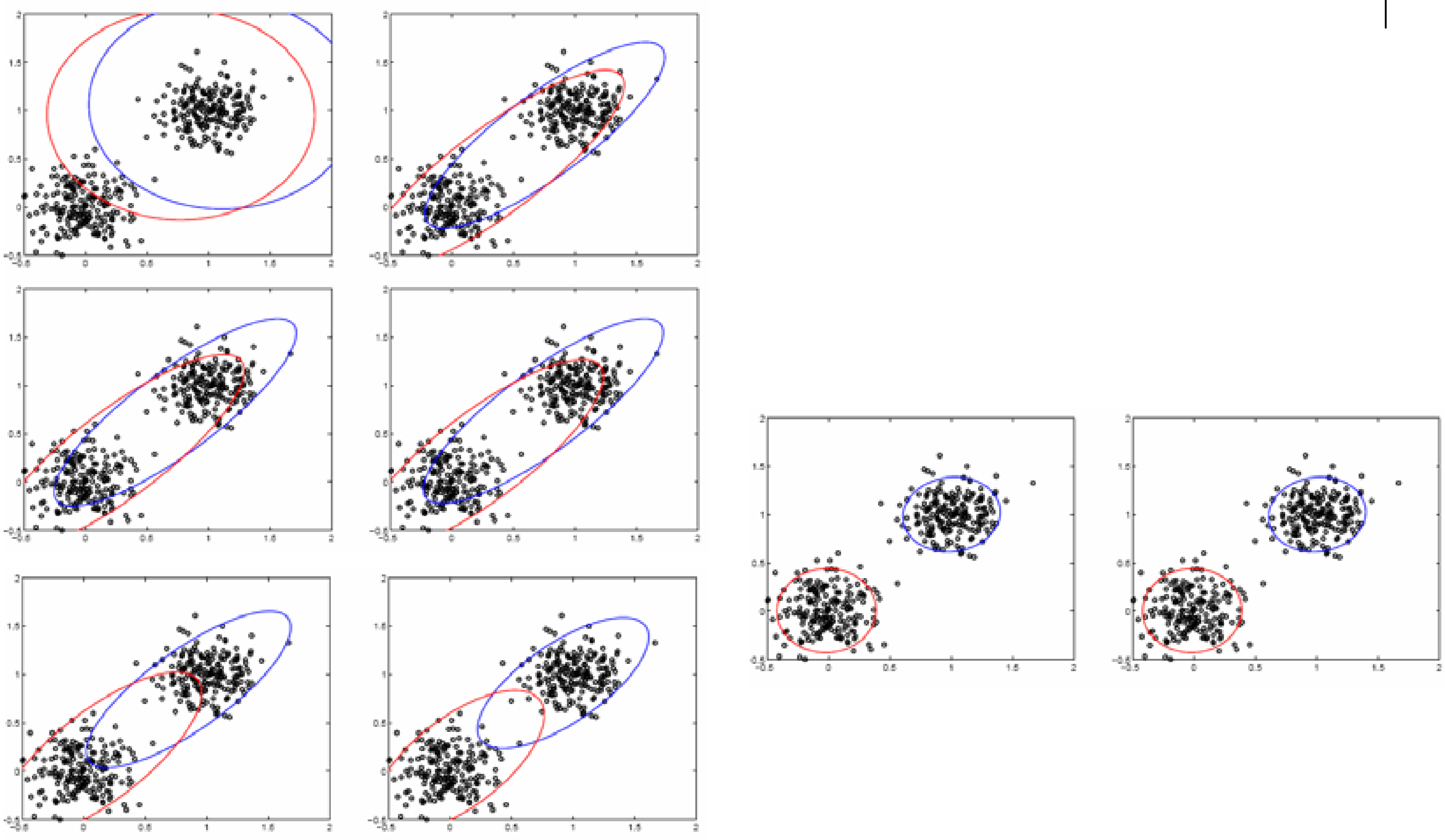


- As a simple strategy for selecting the appropriate number of mixture components, we can find k that minimize the following asymptotic approximation to the description length:

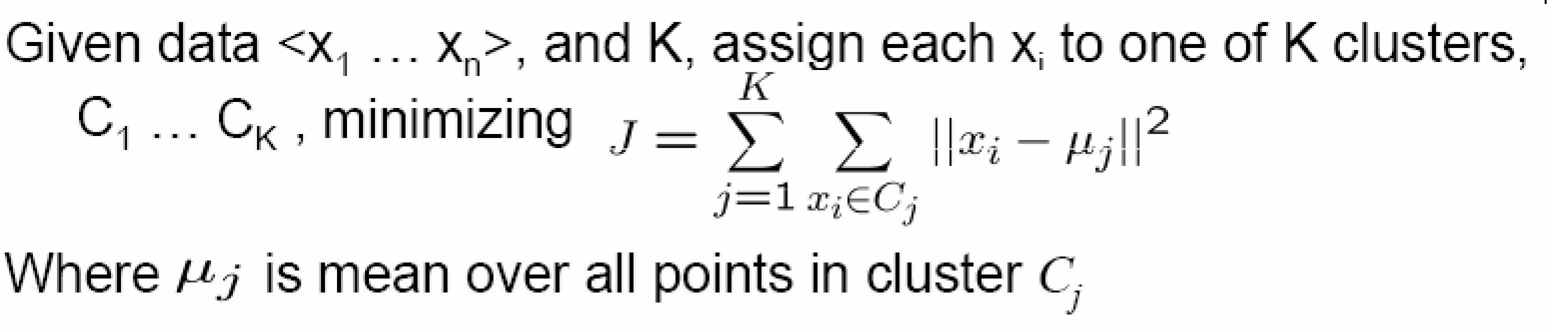
$$\mathrm{DL} \approx -\log p(\mathrm{data}|\hat{\theta}_k) + \frac{d_k}{2}\log(n)$$

where n is the number of training points, $\hat{\theta}_k$ is the maximum likelihood parameter estimate for the k-component mixture, and d_k is the (effective) number of parameters in the k-mixture.

Mixture density estimation: example



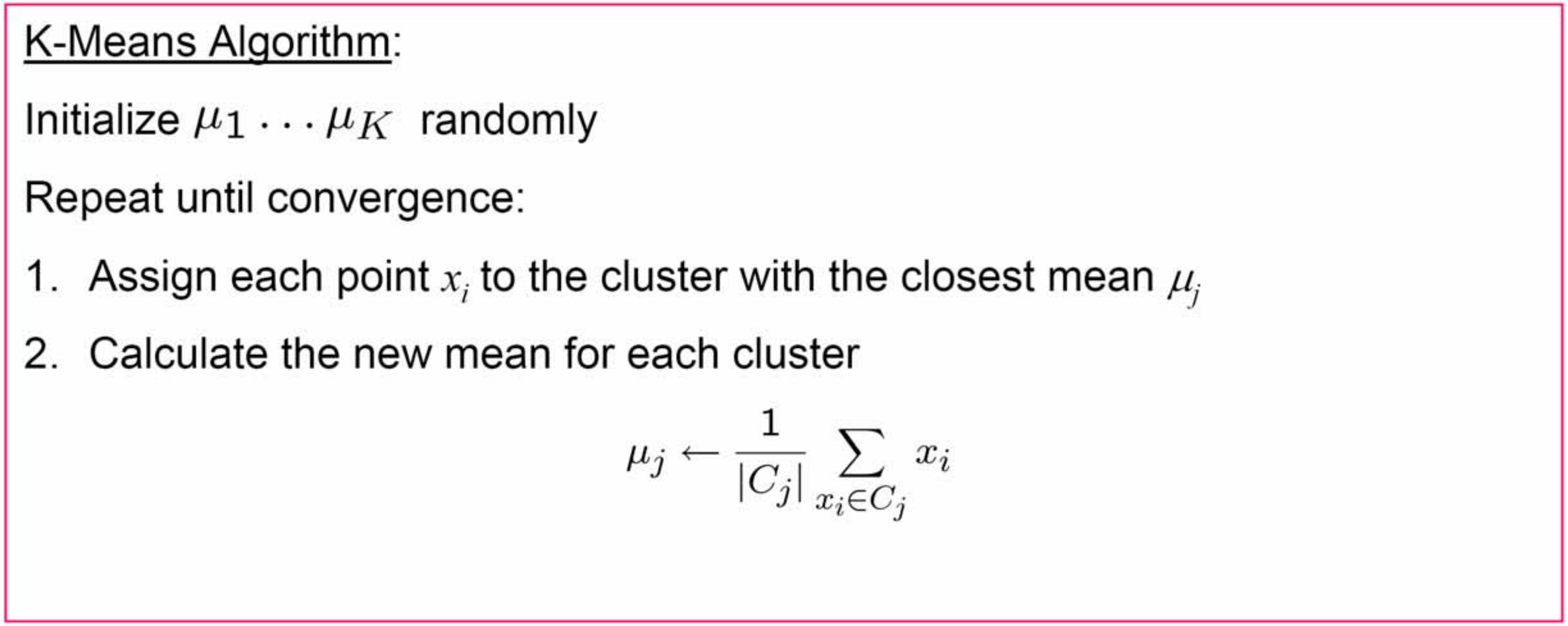
K-means clustering



Given data <x_1 … x_n>, and K, assign each x_i to one of K clusters, C_1 … C_K , minimizing

$$J = \sum_{j=1}^{K} \sum_{x_i \in C_j} ||x_i - \mu_j||^2$$

Where μ_j is mean over all points in cluster C_j



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K-Means Algorithm:
Initialize $\mu_1 \cdots \mu_K$ randomly
Repeat until convergence:
    1. Assign each point $x_i$ to the cluster with the closest mean $\mu_j$
    2. Calculate the new mean for each cluster
           $\mu_j \leftarrow \frac{1}{|C_j|} \sum_{x_i \in C_j} x_i$
```

K-Means vs. Mixture of Gaussians

- Both are iterative algorithms to assign points to clusters

- Objective function
  - K Means: minimize $$J = \sum_{j=1}^{K} \sum_{x_i \in C_j} ||x_i - \mu_j||^2$$
  - MoG: maximize likelihood $P(X|\theta)$

- MoG the more general formulation
  - Equivalent to K Means when $\Sigma_k = \sigma I$, and $\sigma \rightarrow 0$

Hierarchical (bottom-up) clustering

- Hierarchical agglomerative clustering: we sequentially merge the pair of “closest” points/clusters

- The procedure
  1. Find two closest points (clusters) and merge them
  2. Proceed until we have a single cluster (all the points)
- Two prerequisites:
  1. distance measure d(xi, xj) between two points
  2. distance measure between clusters (cluster linkage)

Hierarchical (bottom-up) clustering

- A *linkage* method: we have to be able to measure distances between clusters of examples C_k and C_l

a) Single linkage:

$$d_{kl} = \min_{i \in C_k, j \in C_l} d(\mathbf{x}_i, \mathbf{x}_j)$$

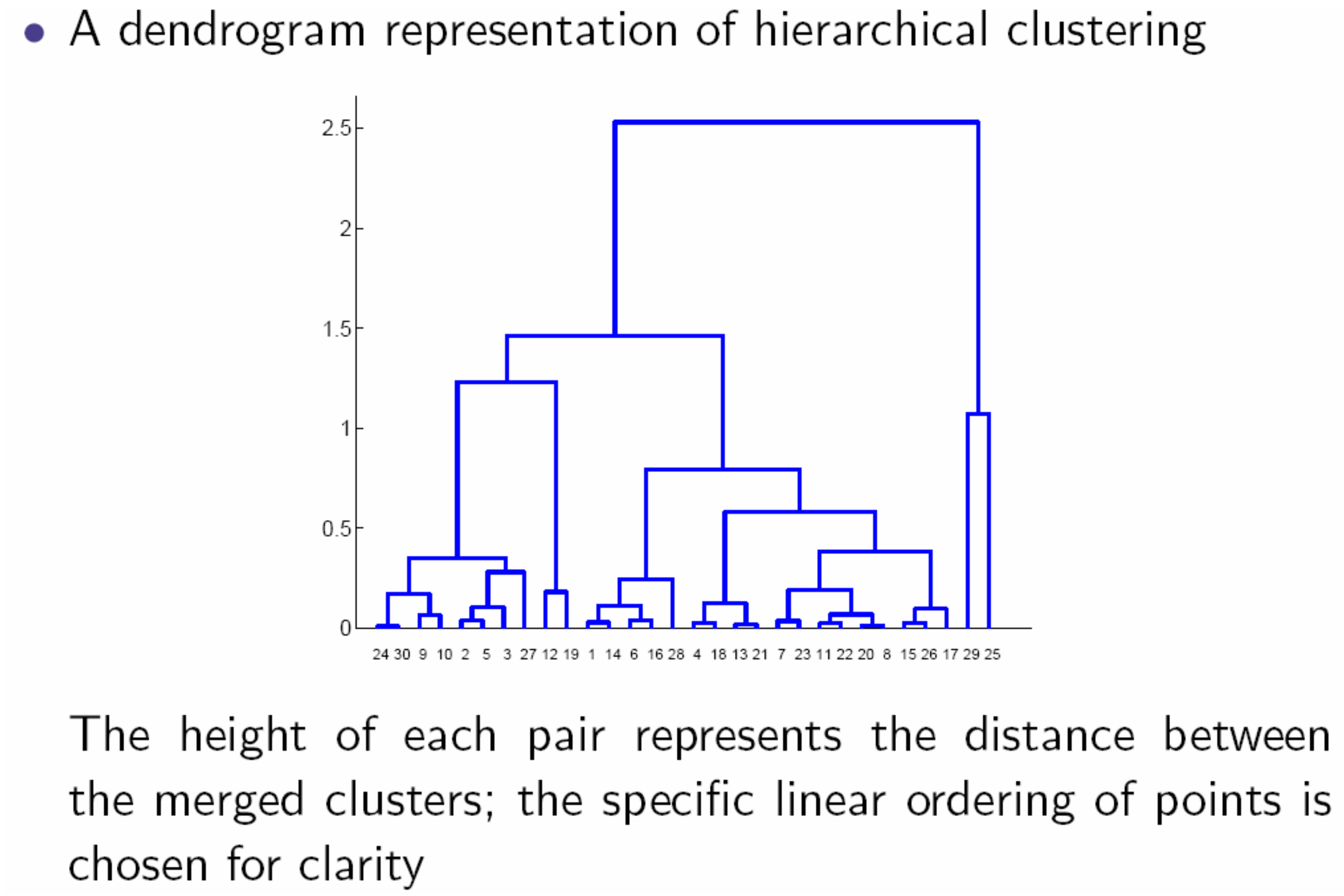
b) Average linkage:

$$d_{kl} = \frac{1}{|C_l|\,|C_k|} \sum_{i \in C_k, j \in C_l} d(\mathbf{x}_i, \mathbf{x}_j)$$

c) Centroid linkage:

$$d_{kl} = d(\bar{\mathbf{x}}_k, \bar{\mathbf{x}}_l), \quad \bar{\mathbf{x}}_l = \frac{1}{|C_l|} \sum_{i \in C_l} \mathbf{x}_i$$

Hierarchical (bottom-up) clustering



- A dendrogram representation of hierarchical clustering

The height of each pair represents the distance between the merged clusters; the specific linear ordering of points is chosen for clarity

Spectral clustering

- The spectral clustering method we define relies on a random walk representation over the points. We construct this in three steps

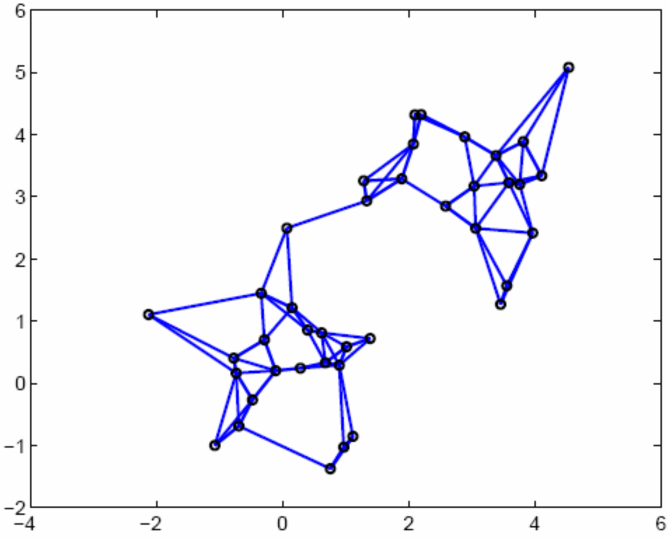
1. a nearest neighbor graph
2. similarity weights on the edges:

$$W_{ij} = \exp\{-\beta\|\mathbf{x}_i - \mathbf{x}_j\|\}$$

   where $W_{ii} = 1$ and the weight is zero for non-edges.

3. transition probability matrix

$$P_{ij} = W_{ij} / \sum_{j'} W_{ij'}$$



Properties of the random walk

- If we start from i_0, the distribution of points i_t that we end up in after t steps is given by

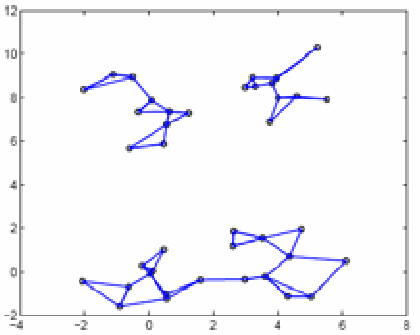
$$i_1 \sim P_{i_0\, i_1}, \qquad P_{ij} = \frac{W_{ij}}{W_{i\cdot}}, \quad \text{where } W_{i\cdot} = \sum_j W_{ij}$$

$$i_2 \sim \sum_{i_1} P_{i_0, i_1} P_{i_1\, i_2} = [P^2]_{i_0\, i_2},$$

$$i_3 \sim \sum_{i_1} \sum_{i_2} P_{i_0, i_1} P_{i_1\, i_2} P_{i_2\, i_3} = [P^3]_{i_0\, i_3},$$

$$\ldots$$

$$i_t \sim [P^t]_{i_0\, i_t}$$

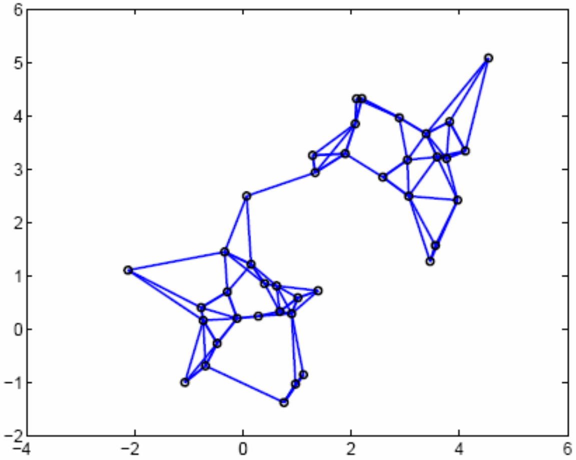


where $P^t = PP\ldots P$ (t matrix products) and $[\cdot]_{ij}$ denotes the i, j component of the matrix.

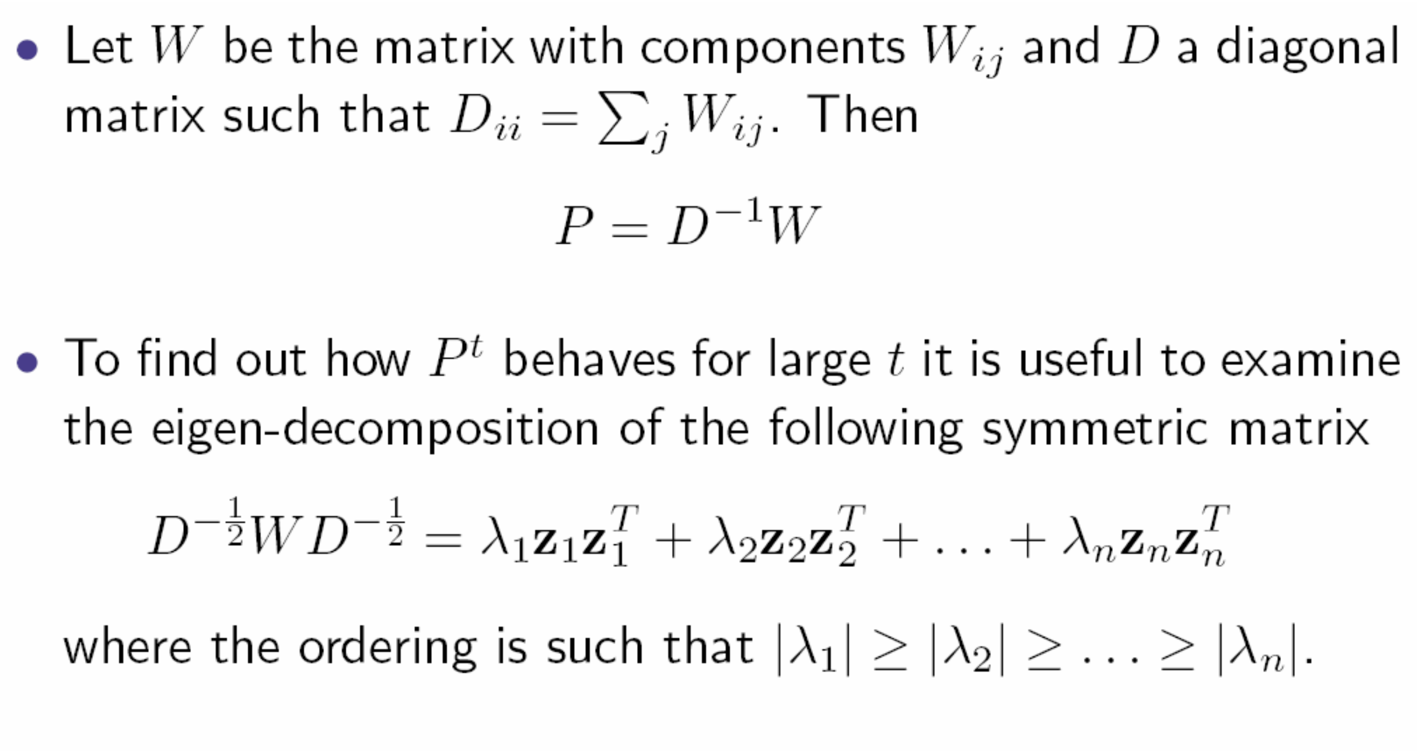
Random walk and clustering

- The distributions of points we end up in after t steps converge as t increases. If the graph is connected, the resulting distribution is independent of the starting point

  Even for large t, the transition probabilities $[P^t]_{ij}$ have a slightly higher probability of transitioning within "clusters" than across; we want to recover this effect from eigenvalues/vectors



Eigenvalues/vectors and spectral clustering



- Let W be the matrix with components W_{ij} and D a diagonal matrix such that $D_{ii} = \sum_j W_{ij}$. Then

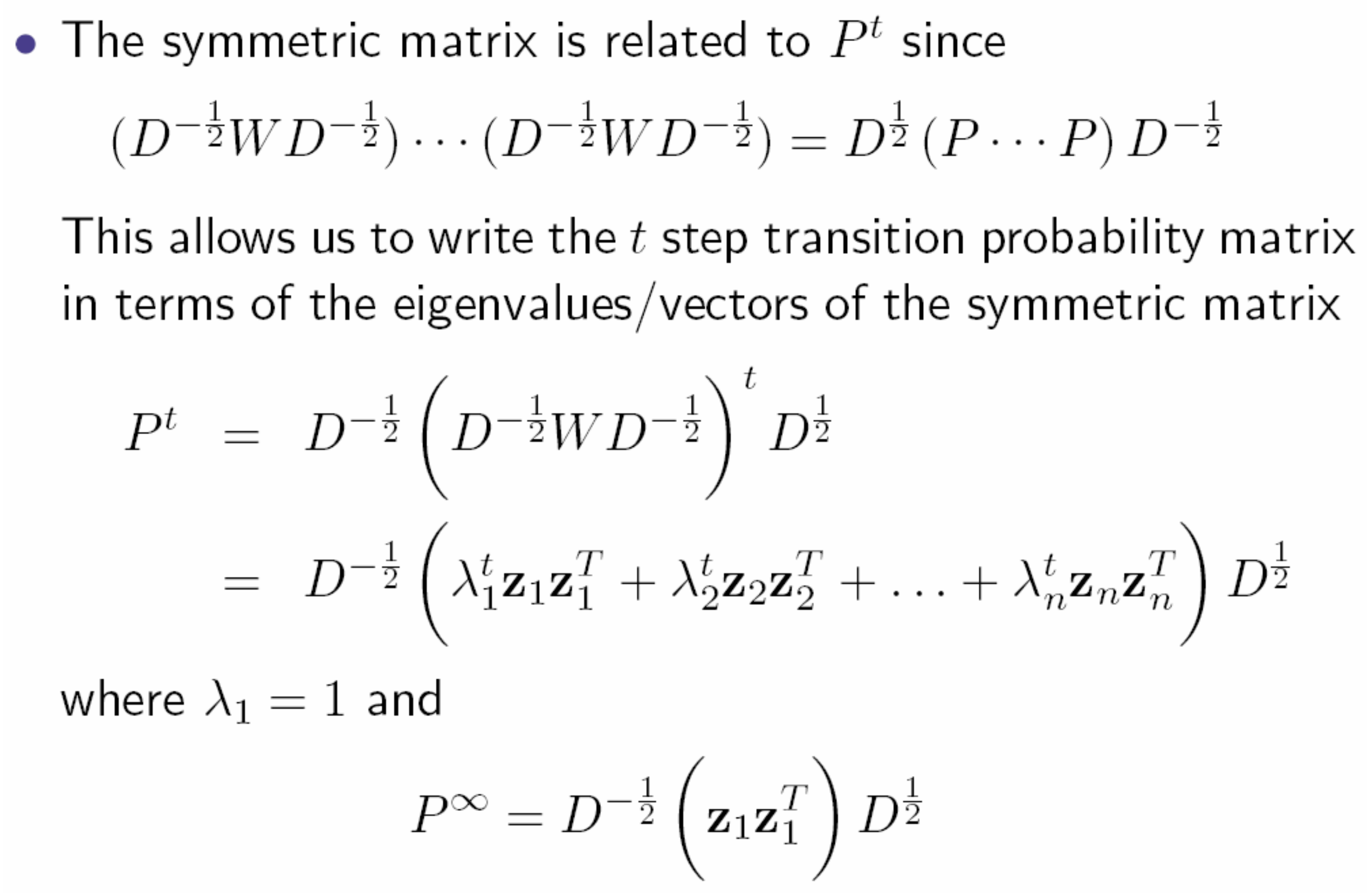
$$P = D^{-1}W$$

- To find out how P^t behaves for large t it is useful to examine the eigen-decomposition of the following symmetric matrix

$$D^{-\frac{1}{2}}WD^{-\frac{1}{2}} = \lambda_1 \mathbf{z}_1 \mathbf{z}_1^T + \lambda_2 \mathbf{z}_2 \mathbf{z}_2^T + \ldots + \lambda_n \mathbf{z}_n \mathbf{z}_n^T$$

where the ordering is such that $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|$.

Eigenvalues/vectors cont'd



- The symmetric matrix is related to P^t since

$$(D^{-\frac{1}{2}}WD^{-\frac{1}{2}})\cdots(D^{-\frac{1}{2}}WD^{-\frac{1}{2}}) = D^{\frac{1}{2}}\left(P\cdots P\right)D^{-\frac{1}{2}}$$

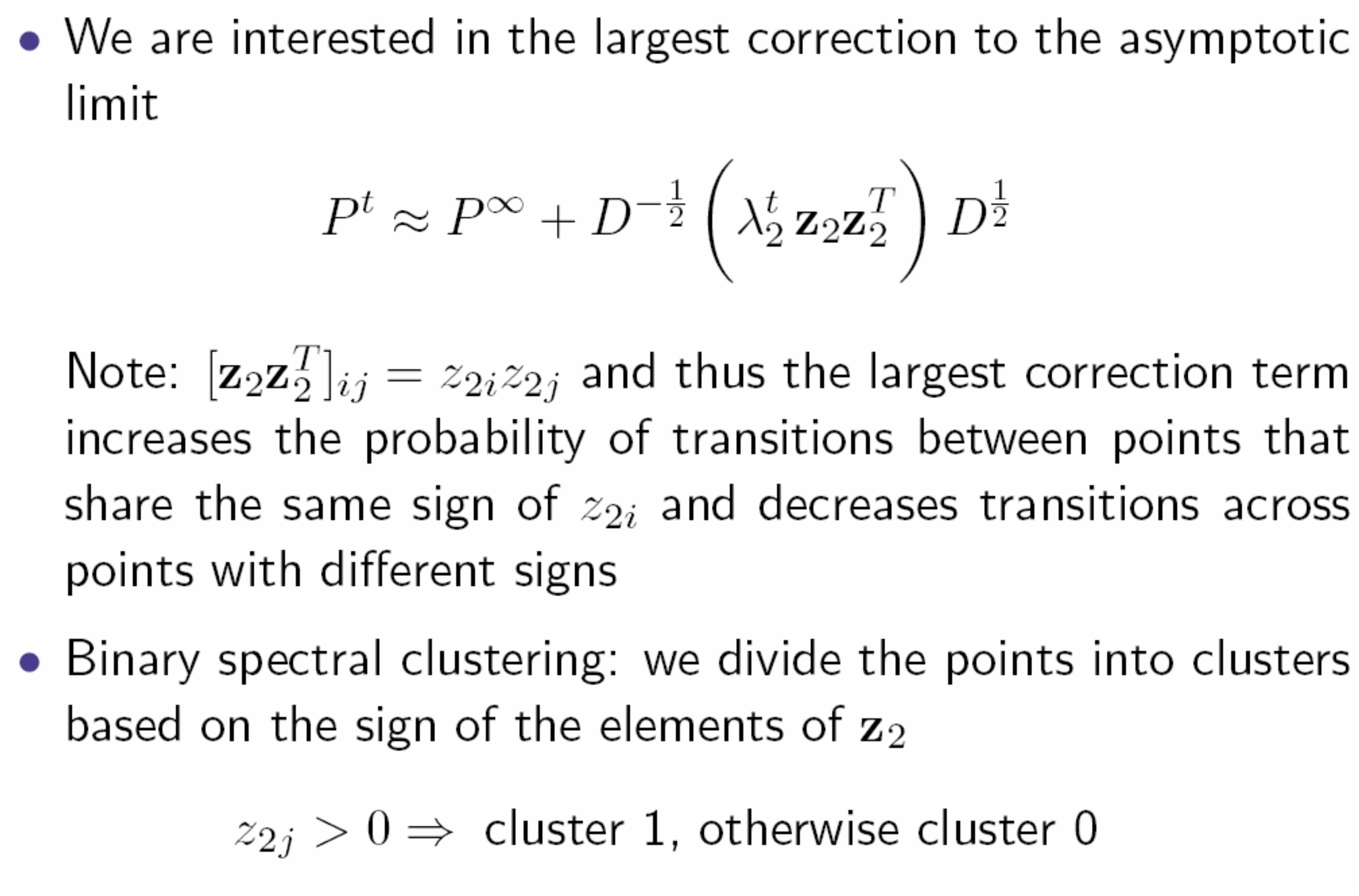
This allows us to write the t step transition probability matrix in terms of the eigenvalues/vectors of the symmetric matrix

$$\begin{aligned} P^t &= D^{-\frac{1}{2}}\left(D^{-\frac{1}{2}}WD^{-\frac{1}{2}}\right)^t D^{\frac{1}{2}} \\ &= D^{-\frac{1}{2}}\left(\lambda_1^t\mathbf{z}_1\mathbf{z}_1^T + \lambda_2^t\mathbf{z}_2\mathbf{z}_2^T + \ldots + \lambda_n^t\mathbf{z}_n\mathbf{z}_n^T\right)D^{\frac{1}{2}} \end{aligned}$$

where $\lambda_1 = 1$ and

$$P^\infty = D^{-\frac{1}{2}}\left(\mathbf{z}_1\mathbf{z}_1^T\right)D^{\frac{1}{2}}$$

Eigenvalues/vectors and spectral clustering



- We are interested in the largest correction to the asymptotic limit

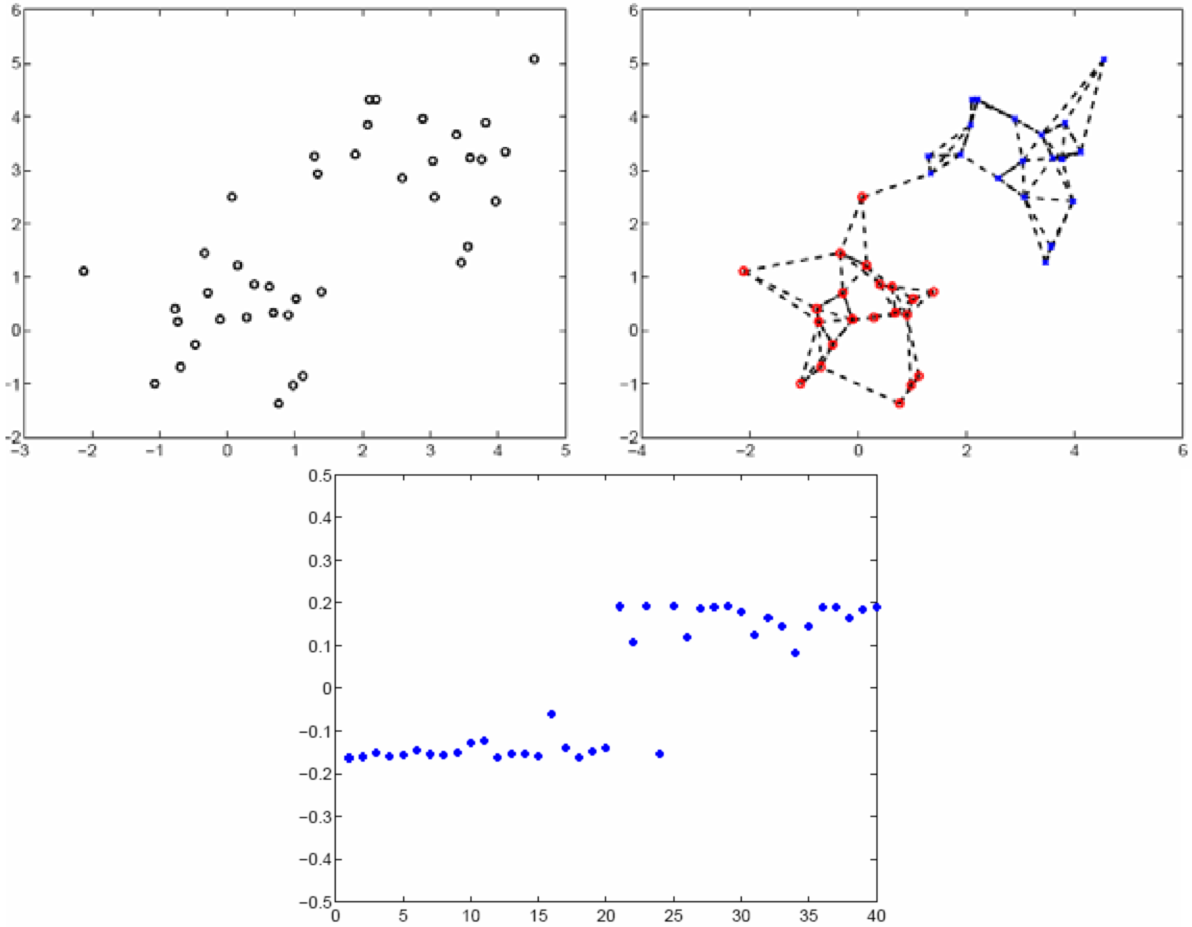
$$P^t \approx P^\infty + D^{-\frac{1}{2}} \left(\lambda_2^t \, \mathbf{z}_2 \mathbf{z}_2^T \right) D^{\frac{1}{2}}$$

Note: $[\mathbf{z}_2 \mathbf{z}_2^T]_{ij} = z_{2i} z_{2j}$ and thus the largest correction term increases the probability of transitions between points that share the same sign of z_{2i} and decreases transitions across points with different signs

- Binary spectral clustering: we divide the points into clusters based on the sign of the elements of $\mathbf{z}_2$

$$z_{2j} > 0 \Rightarrow \text{ cluster 1, otherwise cluster 0}$$

Spectral clustering: example



Components of the eigenvector corresponding to the second largest eigenvalue

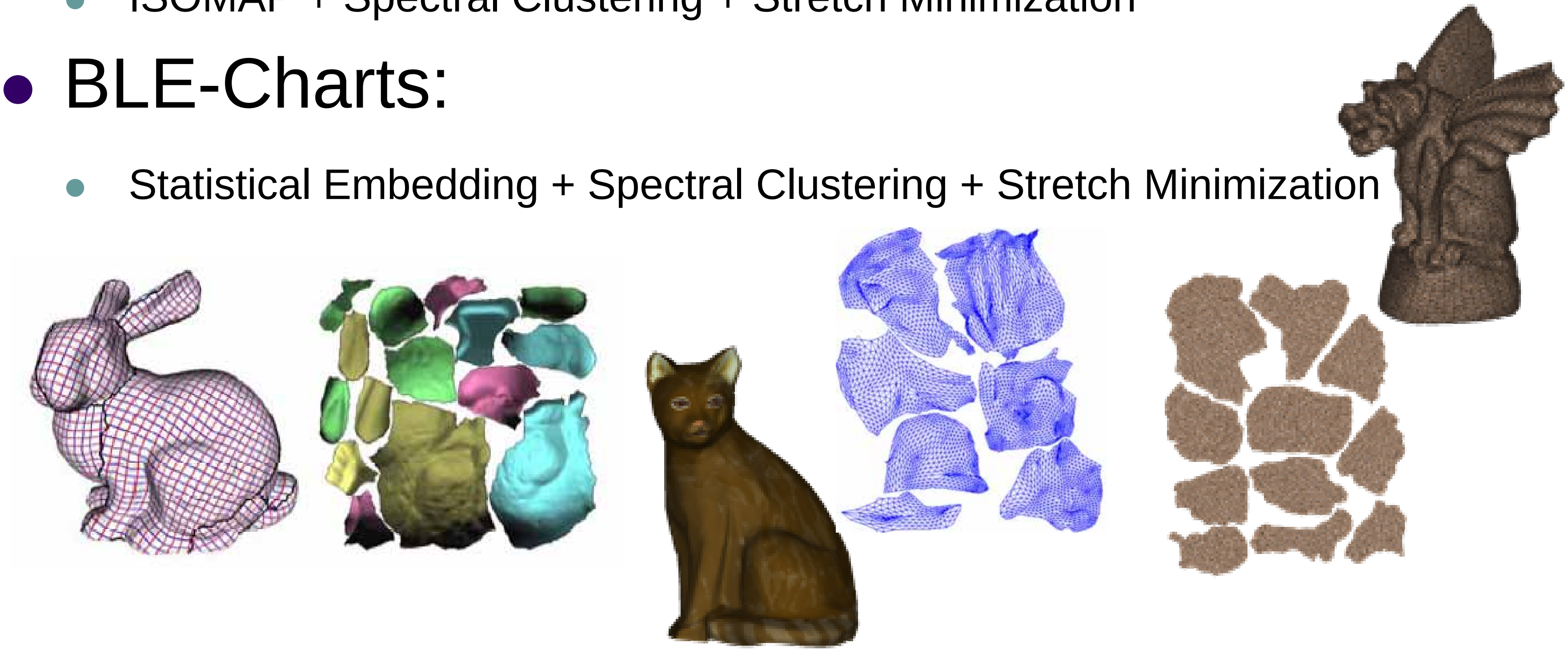
Reference papers of SC

- A. Y. Ng, M. I. Jordan, and Y. Weiss, *On spectral clustering: Analysis and an algorithm*, NIPS, (2001)
- Y. Weiss, *Segmentation using eigenvectors: a unifying view*. ICCV, (1999)
- J. Shi and J. Malik, *Normalized cuts and image segmentation*, IEEE TPAMI, 22 (2000)

- And more about image segmentations …
  - Graph cut
  - Mean-shift

An example: ISO/BLE-charts

- ISO-Charts:
  - ISOMAP + Spectral Clustering + Stretch Minimization
- BLE-Charts:
  - Statistical Embedding + Spectral Clustering + Stretch Minimization



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