**Script** generated by TTT

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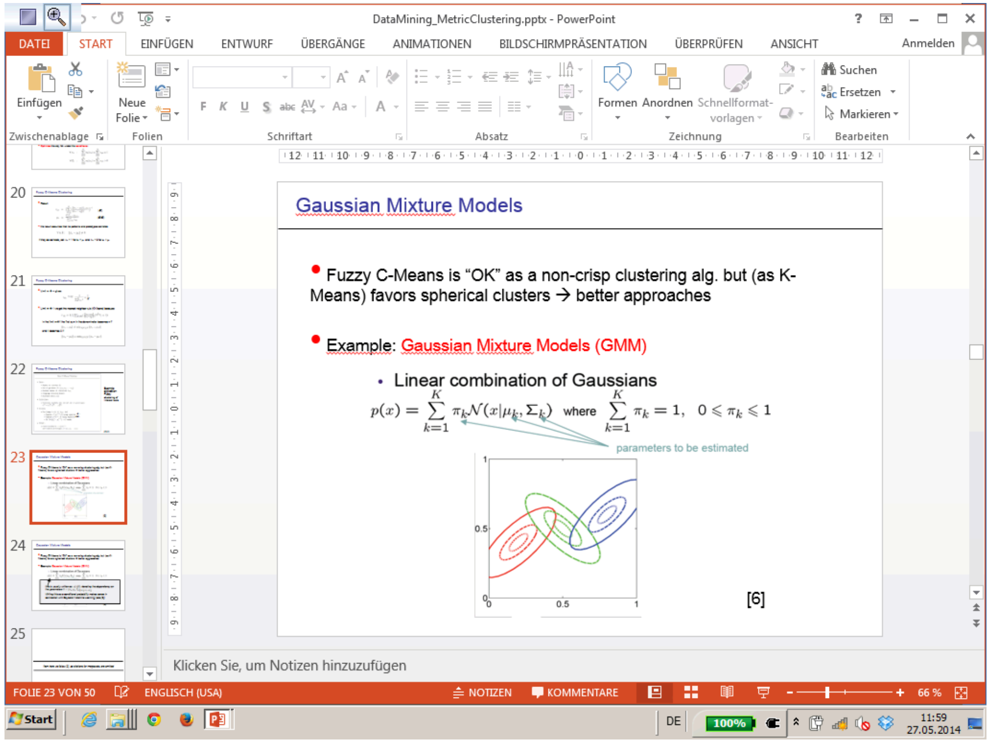


## Gaussian Mixture Models

- Fuzzy C-Means is "OK" as a non-crisp clustering alg. but (as K-Means) favors spherical clusters → better approaches
- Example: Gaussian Mixture Models (GMM)
  - Linear combination of Gaussians

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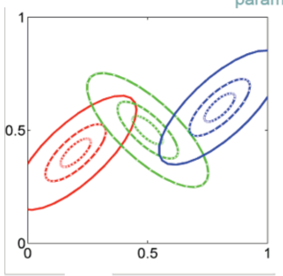
parameters to be estimated




[6]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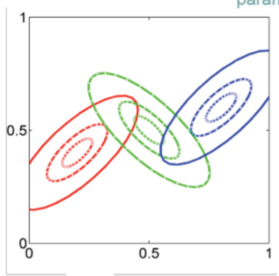

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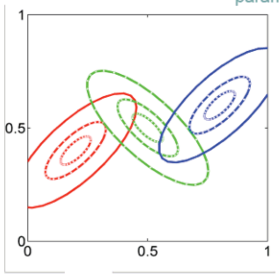


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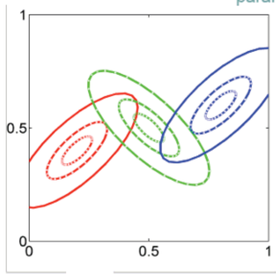

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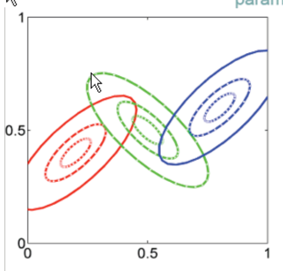

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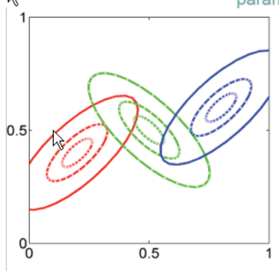

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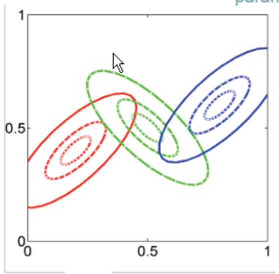


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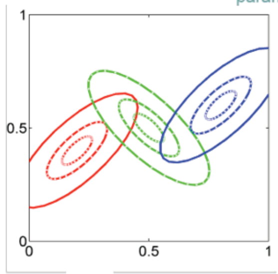


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# Machine Learning

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Example: $x \in \mathbb{R}^n$ and $p(x|\Theta)$ is one multivariate Gaussian)

$$p(\mathbf{x}|\Theta) = \mathcal{N}(\mathbf{x}|\underbrace{\boldsymbol{\mu}, \boldsymbol{\Sigma}}_{\theta}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

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$$\ln\, p(\mathbf{X}|\Theta) = \ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu})$$

- Maximum log likelihood:

$$\Theta_{ML} = argmax_{\Theta}\ \log p(X|\Theta) \Rightarrow \nabla_{\Theta}\left(\textstyle\sum_i \log p(x_i|\Theta)\right) \overset{!}{=} 0$$

$$\left.\begin{aligned} \boldsymbol{\mu}_{\mathrm{ML}} &: \frac{\partial}{\partial \boldsymbol{\mu}} \ln p(\mathbf{X}\,|\,\mu, \boldsymbol{\Sigma}) = 0 \\ \boldsymbol{\Sigma}_{\mathrm{ML}} &: \frac{\partial}{\partial \boldsymbol{\Sigma}} \ln p(\mathbf{X}\,|\,\boldsymbol{\mu}, \boldsymbol{\Sigma}) = 0 \end{aligned}\right\} \Rightarrow \begin{aligned} \boldsymbol{\mu}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n \\ \boldsymbol{\Sigma}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})^{\mathrm{T}} \end{aligned}$$


## Machine Learning

Example: $x \in \mathbb{R}^n$ and $p(x|\Theta)$ is one multivariate Gaussian)

$$p(\mathbf{x}|\Theta) = \mathcal{N}(\mathbf{x}|\underbrace{\boldsymbol{\mu}, \boldsymbol{\Sigma}}_{\theta}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

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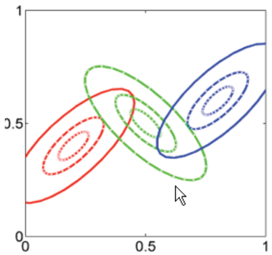

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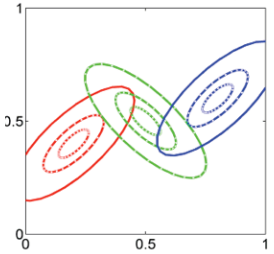


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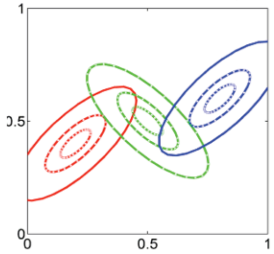


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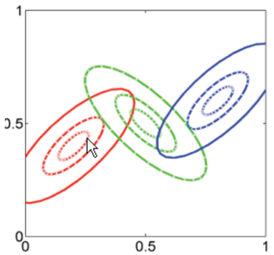


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- **1 of K representation**

  $K$-dimensional binary random variable $\mathbf{z}$

  $z_k \in \{0, 1\}$ and $\sum_k z_k = 1$

  $p(z_k = 1) = \pi_k$

  $$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}$$

- **conditional probability**

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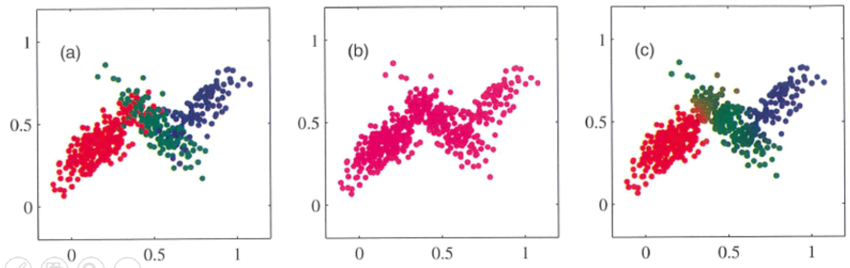
- Example

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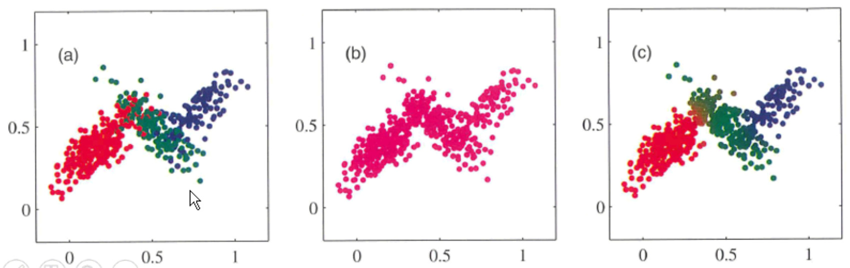


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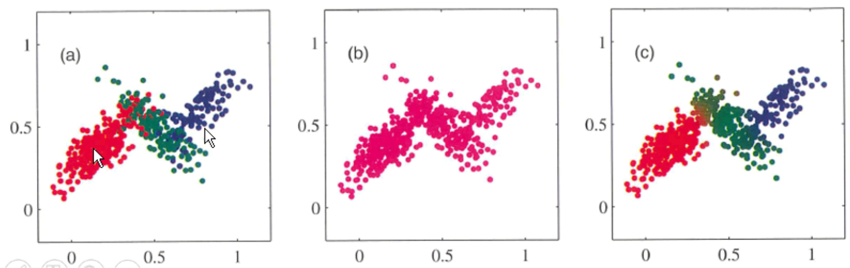

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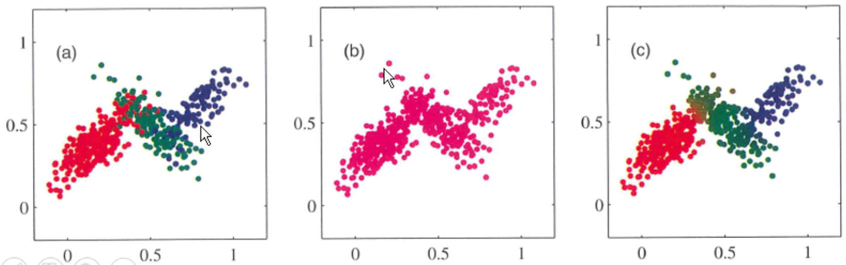



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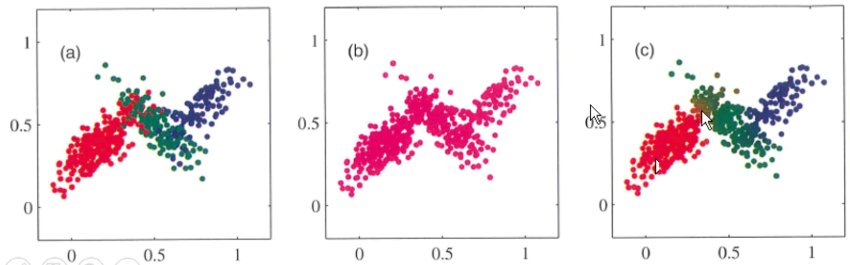



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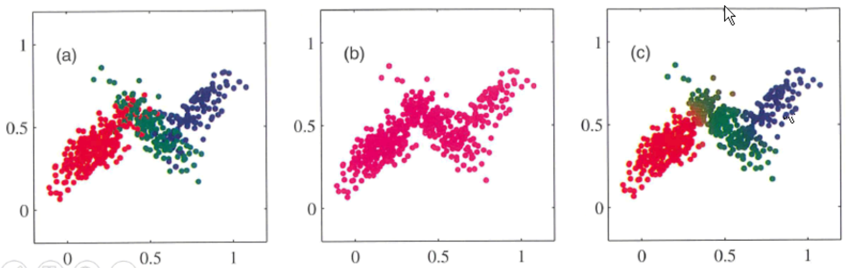


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Maximum likelihood (GMM)

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Vector of $K$ $D$-dim. means $\boldsymbol{\mu}_k$

Vector of $K$ $DxD$ covariances $\boldsymbol{\Sigma}_k$

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$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \qquad \boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

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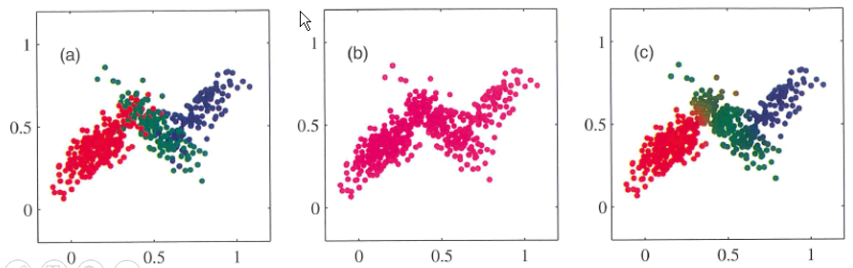

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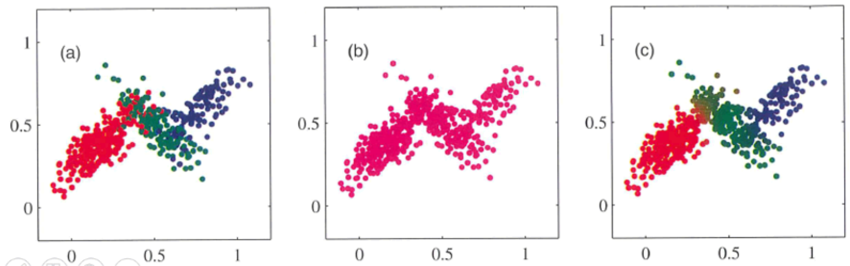


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### Maximum likelihood (GMM)

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

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Vector of $K$ *DxD* covariances $\boldsymbol{\Sigma}_{\mathrm{k}}$

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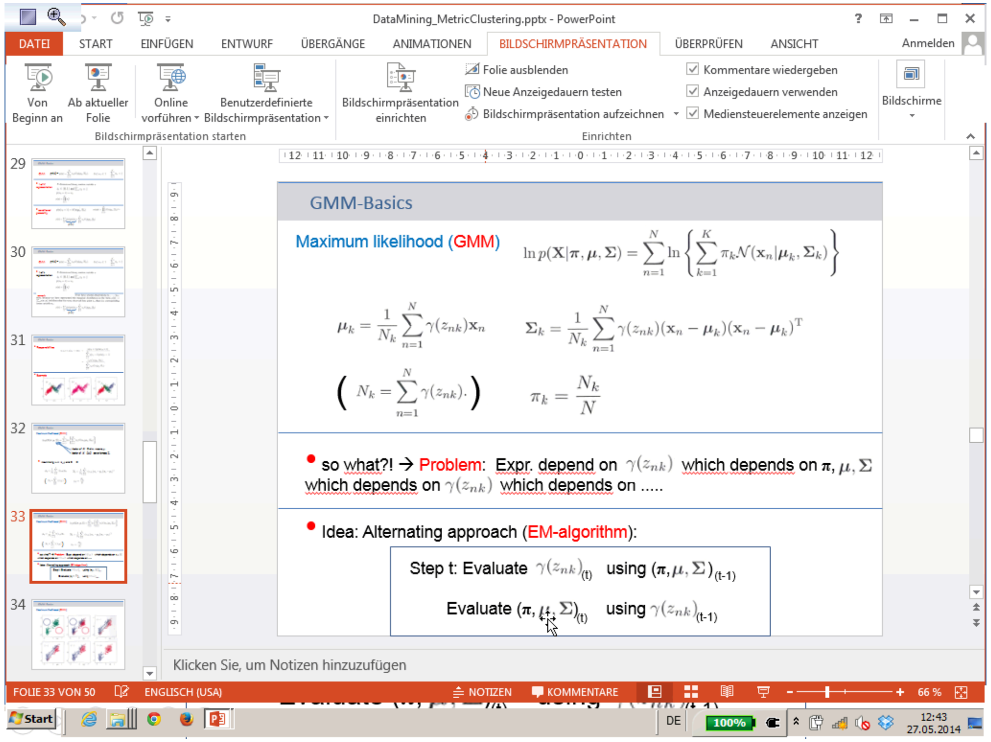



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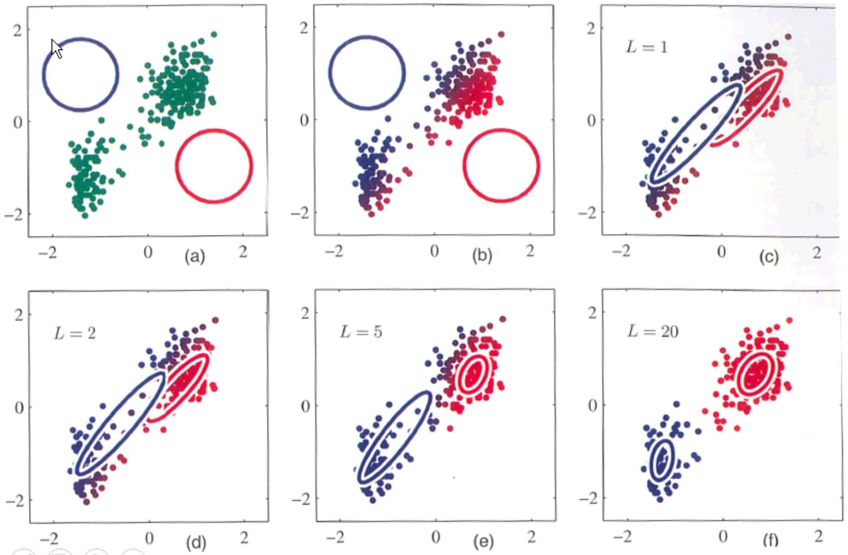



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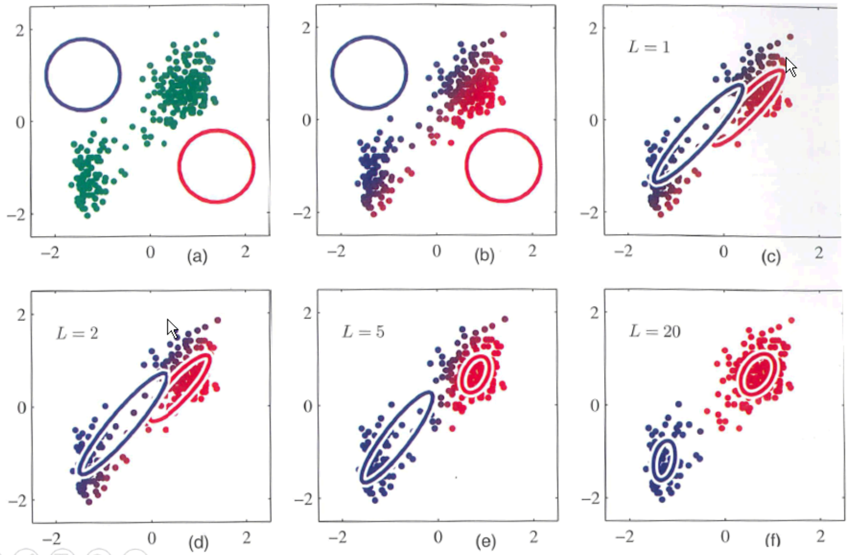

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**EM for Gaussian Mixtures**

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing coefficients).

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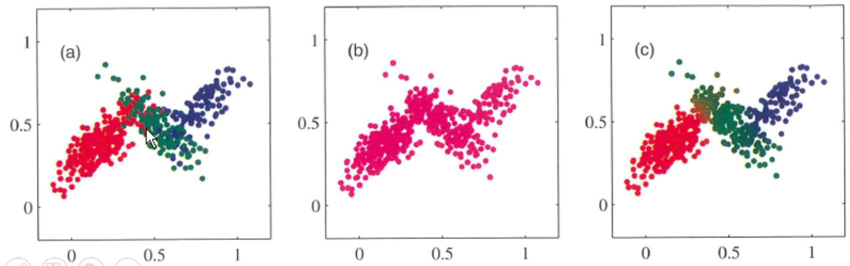
## GMM-Basics

- Responsibilities

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

- Example



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- alternating EM:

E-Step: compute
$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}).$$

M-Step: compute
$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}).$$


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*that is why K-Means favors spherical clusters*

- If we use k Gaussians with Σ = εI:

$$p(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) = \frac{1}{(2\pi\epsilon)^{1/2}} \exp\left\{-\frac{1}{2\epsilon}\|\mathbf{x}-\boldsymbol{\mu}_k\|^2\right\}$$

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## Real World Networks: Properties and Models

Lecture will mostly follow [1], thus corresponding citations are often omitted to increase readability

## Information Networks / Knowledge NW

- Most studied examples: citation NW (tree), the WWW;
- Example findings:
  - p(k) of author having k papers: $p(k) \sim k^{-\alpha}$ : power law
  - distribution of in or out degrees of WWW pages (also for citation NW): $p(k) \sim k^{-\alpha}$

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- Other examples:
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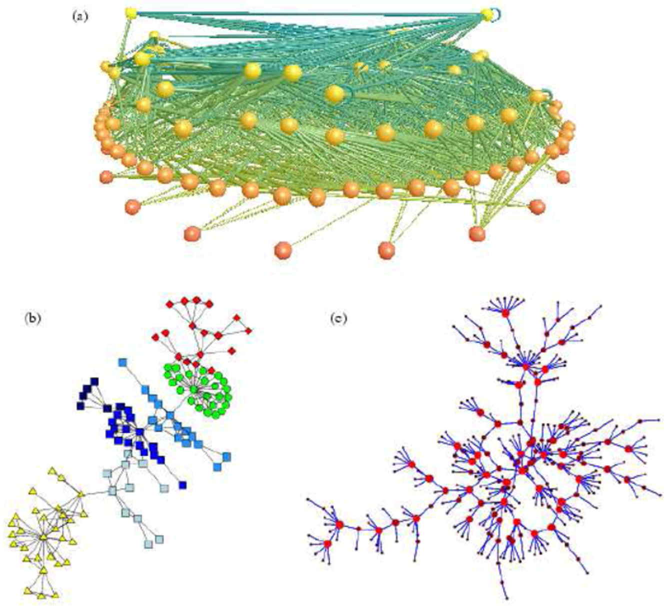


FIG. 2 Three examples of the kinds of networks that are the topic of this review. (a) A food web of predator-prey interactions between species in a freshwater lake [272]. Picture courtesy of Neo Martinez and Richard Williams. (b) The network of collaborations between scientists at a private research institution [171]. (c) A network of sexual contacts between individuals in the study by Potterat *et al.* [342].

[1]

## Mean Average Path Length

- "Small World Effect": $l(n)$ "small" → $l(n) \in O(log(n))$
- undirected graph:

$$\ell = \frac{1}{\frac{1}{2}n(n+1)} \sum_{i \geq j} d_{ij}$$

formula also counts 0 distances from i to i: ½ n(n+1) = ½ n(n-1) + n

- Expression allowing for disconnected components (where $d_{ij}=\infty$ can occur): harmonic mean:

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## Transitivity / Clustering Coefficient

- Clustering coefficient (whole graph):

$$C = C^{(1)} = \frac{3\times \text{ number of triangles in the network}}{\text{number of connected triples of vertices}} = \frac{6\times \text{ number of triangles in the network}}{\text{number of paths of length two}}$$

p(FOAF)

- Clustering coefficient (Watts-Strogatz-version, for node i):

$$C_i = \frac{\text{number of triangles connected to vertex } i}{\text{number of triples centered on vertex } i} = \frac{|\{e_{\{kj\}} \mid v_k, v_j \in N_i\}|}{\frac{k_i(k_i-1)}{2}}$$

(see Introduction , $k_i$ = degree of node i)

Clustering coefficient (Watts-Strogatz-version, for whole graph):

$$C = C^{(2)} = \frac{1}{n}\sum_i C_i$$

mean of ratio instead of ratio of means

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