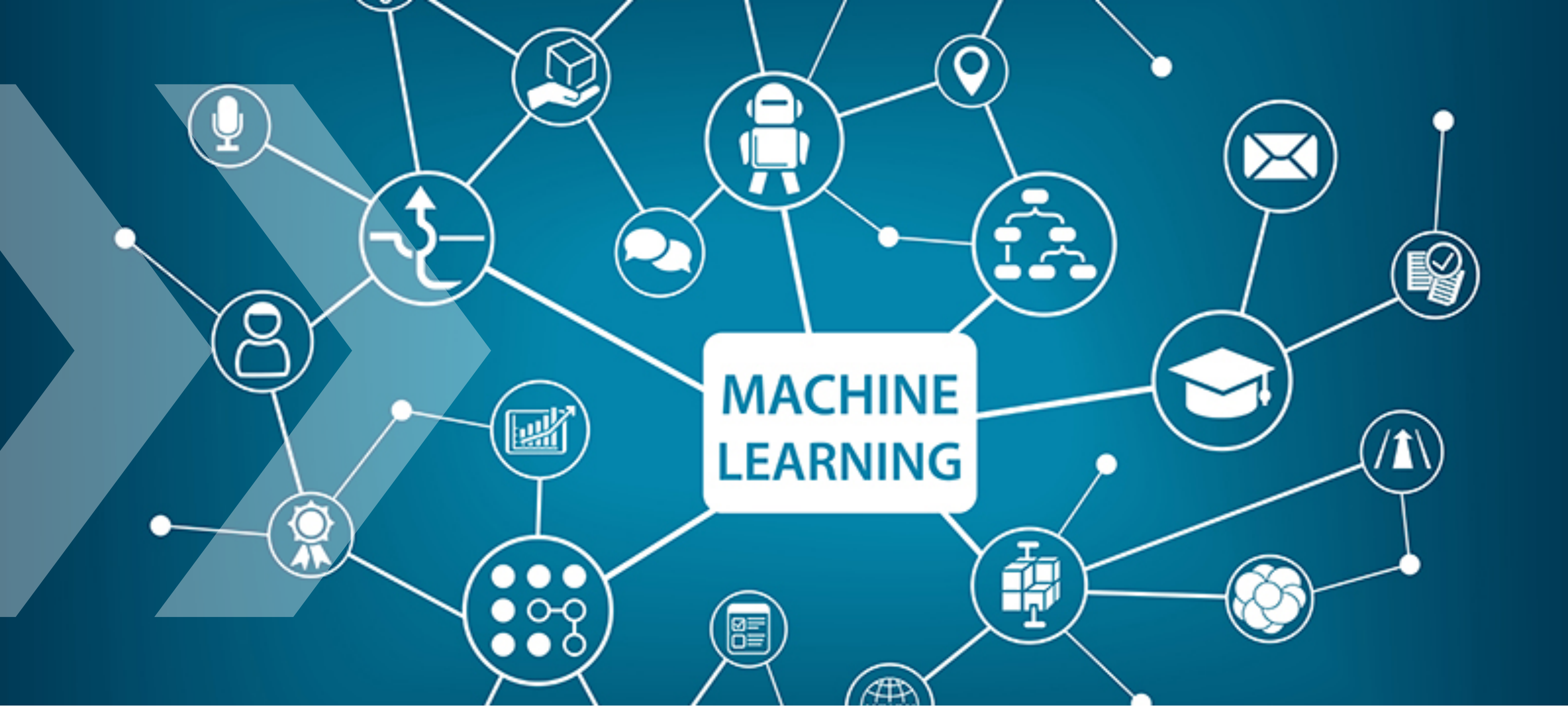
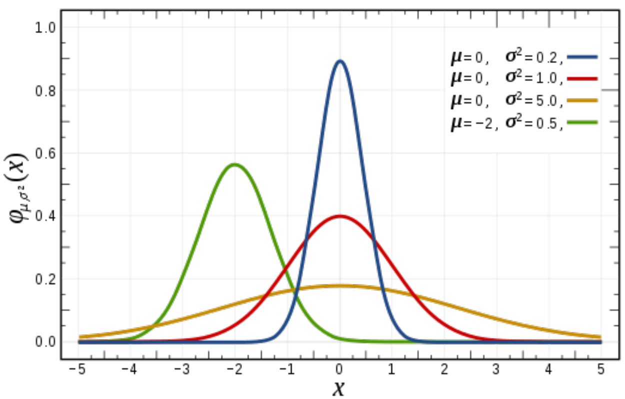


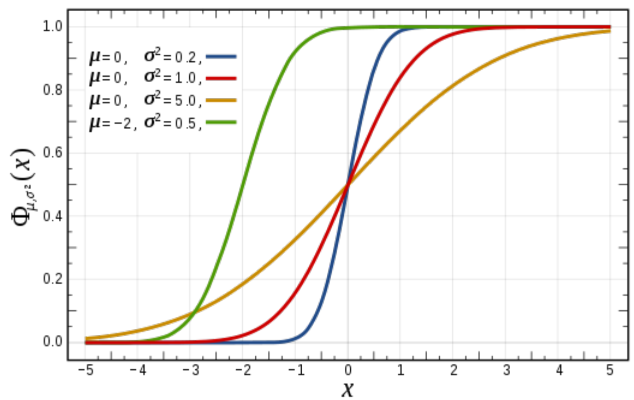
CS489/698: Intro to ML

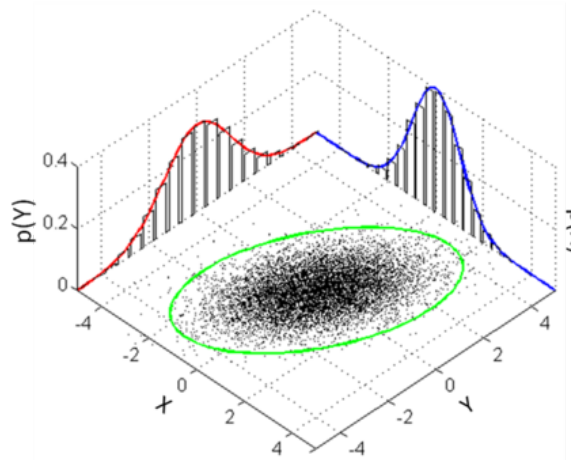
Lecture 10: Mixture of Gaussians

UNIVERSITY OF WATERLOO

Recap: Gaussian distribution



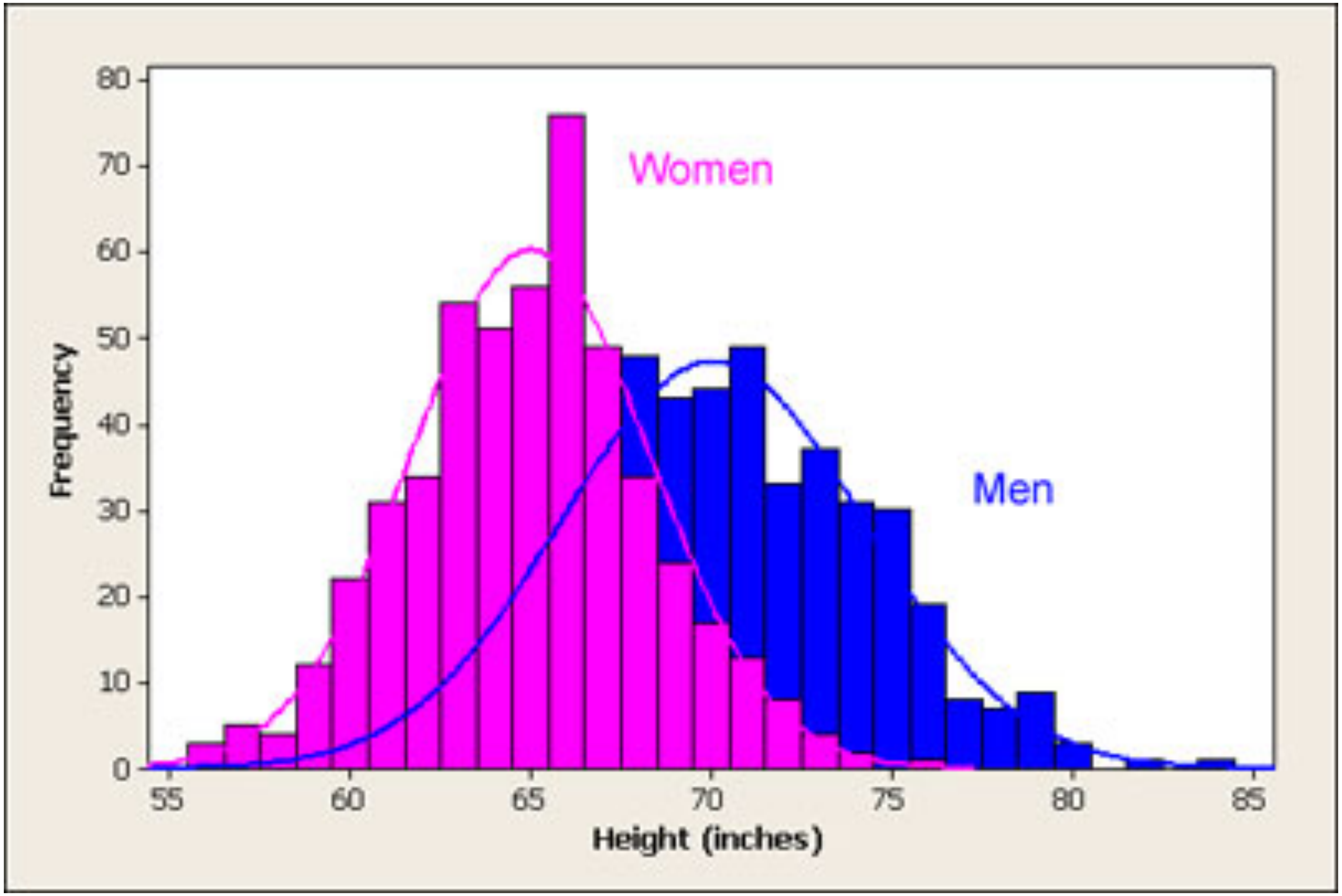




$$p(\mathbf{x}) = (2\pi)^{-d/2}|S|^{-1/2}\exp\left[-\tfrac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top S^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

UNIVERSITY OF WATERLOO

Multi-modality



UNIVERSITY OF WATERLOO

Mixture models

$$\underbrace{p(x|\theta)}_{\text{parameters}} = \sum_{k=1}^{\overset{K}{\text{\# of components}}} \underbrace{p(z=k)}_{\substack{\pi_k \\ \text{mixing distr.}}} \underbrace{p(x|z=k,\theta)}_{\substack{p_k(x|\theta) \\ \text{k-th component distr.}}}$$

$$\pi_k \geq 0, \sum_k \pi_k = 1$$

- Where did we see a similar idea?

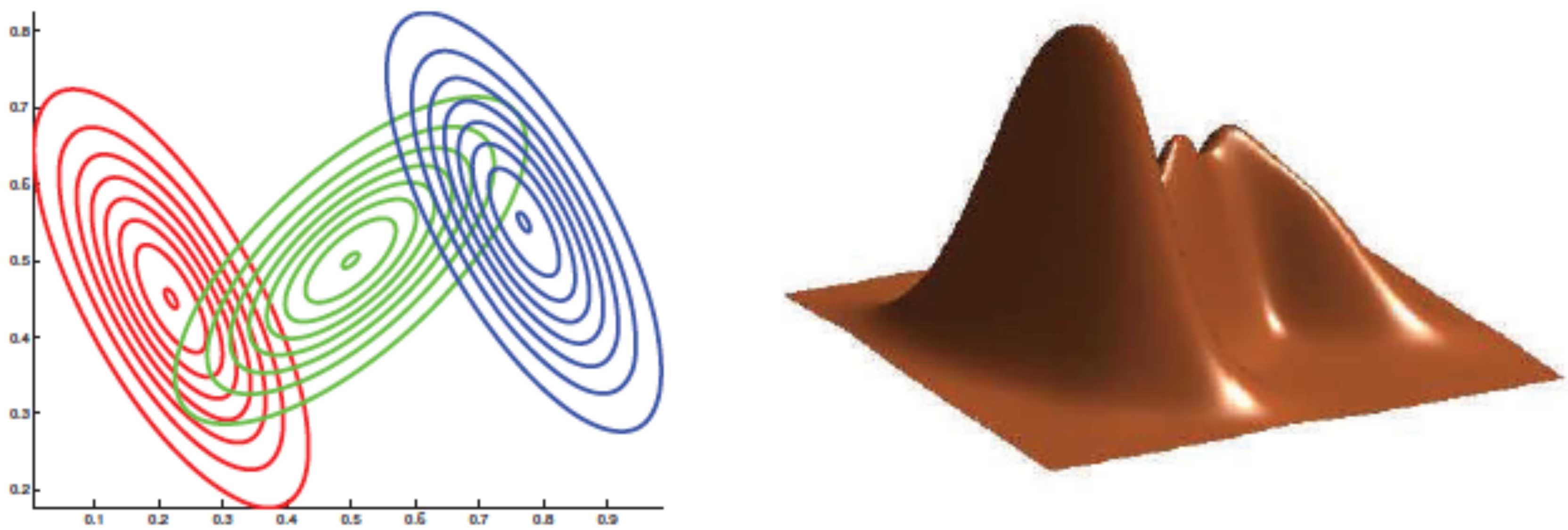
UNIVERSITY OF WATERLOO

Example: Gaussian Mixture Models

$(\pi, \mu_1, S_1, \mu_2, S_2, \ldots, \mu_K, S_K)$

$\|$

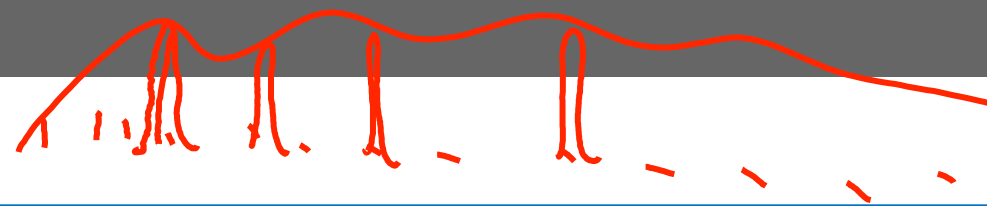
$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, S_k)$$



(a) (b)

UNIVERSITY OF WATERLOO

Universality $e^{-\frac{(x-\mu)^2}{2\sigma^2}}$



Theorem. GMM with sufficiently many components can approximate any probability density function on R^d.

- How many is many?
- Nothing special about Gaussian here, except computationally (later).

Example: Mixture of Experts

$$\frac{\exp(\mathbf{x}^\top \mathbf{v}_k)}{\sum_{c=1}^{K} \exp(\mathbf{x}^\top \mathbf{v}_c)}$$

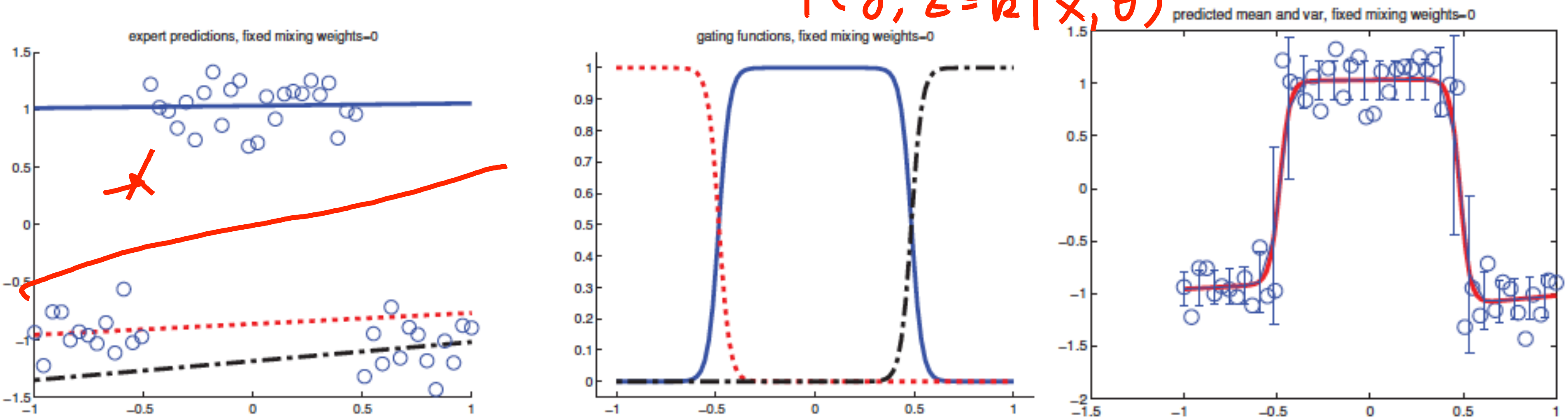
Where did we see a similar idea?

$$\mathcal{N}(y|\mathbf{w}_k^\top \mathbf{x}, \sigma_k^2)$$

mixing distr.

k-th component distr.

$$p(y|\mathbf{x},\boldsymbol{\theta}) = \sum_{k=1}^{K} \underbrace{p(z=k|\mathbf{x},\boldsymbol{\theta})p(y|\mathbf{x},z=k,\boldsymbol{\theta})}_{p(y,z=k|x,\theta)}$$



(a) (b) (c)

Inference problem

$$p(x|\boldsymbol{\theta}) = \sum_{k=1}^{K} p(z = k)p(x|z = k, \boldsymbol{\theta})$$

latent (unobserved)

- Given iid sample $X_1, X_2, \ldots, X_n$ from $p(x|\theta)$
- Need to estimate θ
- Maximum likelihood is NP-hard…

Soft clustering

$$p(z = k | \mathbf{x}, \boldsymbol{\theta}) = \frac{p(z = k | \boldsymbol{\theta}) p(\mathbf{x} | z = k, \boldsymbol{\theta})}{\sum_{c=1}^{K} p(z = c | \boldsymbol{\theta}) p(\mathbf{x} | z = c, \boldsymbol{\theta})}$$

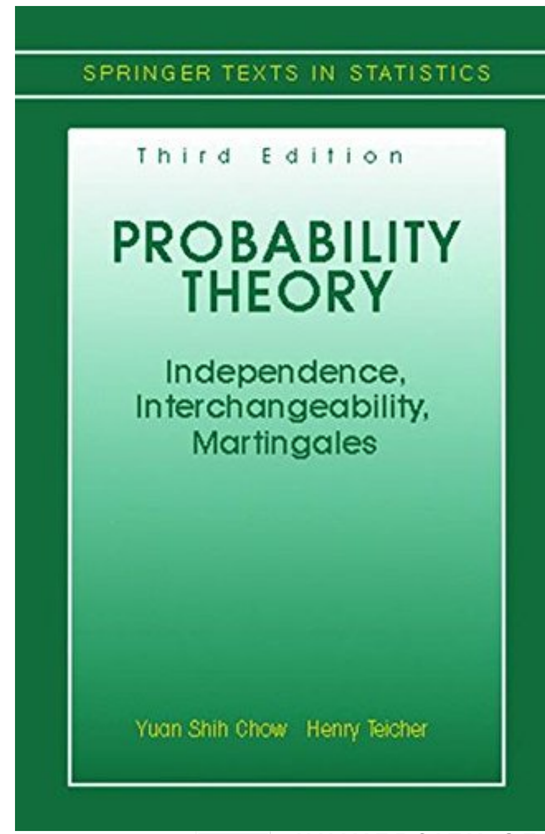
(Stauffer & Grimson, CVPR'98)

Bigger issue: identifiability?

$$p(x|\boldsymbol{\theta}) = \sum_{k=1}^{K} p(z=k) p(x|z=k, \boldsymbol{\theta})$$

- Is this factorization even unique?

- Yes, for GMMs!



Variational form of Max Likelihood

$$\min_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) := \sum_{i=1}^{n} -\log p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{i=1}^{n} -\underbrace{\log \sum_{z_i} p(\mathbf{x}_i, z_i|\boldsymbol{\theta})}_{=}$$

$$\min_{q_i(z_i)\geq 0, \sum_{z_i} q_i(z_i)=1} -\sum_{z_i} q_i(z_i) \log p(\mathbf{x}_i, z_i|\boldsymbol{\theta}) + \underbrace{\sum_{z_i} q_i(z_i) \log q_i(z_i)}_{\text{neg. entropy}}$$

$$\sum_{z_i} q_i(z_i) \log \frac{q_i(z_i)}{p(x_i,z_i|\theta)/\sum_{z_i} p(x_i,z_i|\theta)} \quad \sum_{z_i} p(x_i,z_i|\theta)$$

$$\min_{q_i(z_i)} \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left[\sum_{z_i} q_i(z_i) \log q_i(z_i) - \sum_{z_i} q_i(z_i) \log p(\mathbf{x}_i, z_i|\boldsymbol{\theta}) \right]$$

$$\sum_{z_i} q_i(z_i) \log \frac{1}{\sum_{z_i} p(x_i,z_i|\theta)}$$

KL divergence

$$\mathsf{KL}(\mathbf{p}\|\mathbf{q}) := \sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right) \geq 0$$

Jensen's inequality
E(log(X)) <= log(E(X))

- Both **p** and **q** are nonnegative and sum to 1
- Equality holds iff **p == q**
- Measures difference between distributions; asymmetric

The EM algorithm

$$\min_{q_i(z_i)} \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left[\sum_{z_i} q_i(z_i) \log q_i(z_i) - \sum_{z_i} q_i(z_i) \log p(\mathbf{x}_i, z_i | \boldsymbol{\theta}) \right]$$

- Fix q, solve θ

$$\boxed{\min_{\boldsymbol{\theta}} - \sum_{i=1}^{n} \sum_{z_i} q_i(z_i) \log p(\mathbf{x}_i, z_i | \boldsymbol{\theta})}$$

often closed-form

- Fix θ, solve q

$p(z_i|x_i;\theta)\cdot p(x_i|\theta)$

$\|$

$$\min_{q_i(z_i) \geq 0, \sum_{z_i} q_i(z_i) = 1} \underbrace{- \sum_{z_i} q_i(z_i) \log p(\mathbf{x}_i, z_i | \boldsymbol{\theta}) + \sum_{z_i} q_i(z_i) \log q_i(z_i)}_{KL(q_i \| p(z_i|x_i,\theta))}$$

$- \log(p(x_i|\theta))$

$$\boxed{q_i(z_i) = p(z_i | \mathbf{x}_i, \boldsymbol{\theta})}$$

UNIVERSITY OF WATERLOO

EM for GMM: step 1

$q_i(z_i = k) = r_{ik} \geq 0$

$\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, S_k)$

$$\min_{r_{ik} \geq 0, \sum_k r_{ik} = 1} \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left[\sum_{k=1}^{K} r_{ik} \log r_{ik} - \sum_{k=1}^{K} r_{ik} \log p(\mathbf{x}_i, z_i | \boldsymbol{\theta}) \right]$$

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \sum_{k=1}^{K} r_{ik} [- \log \pi_k + \tfrac{1}{2} \log |S_k| + \tfrac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top S_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)]$$

$$\boxed{\pi_k = \frac{\sum_i r_{ik}}{n}} = \sum_k \sum_i r_{ik} \qquad \boxed{\boldsymbol{\mu}_k = \frac{\sum_{i=1}^{n} r_{ik} \mathbf{x}_i}{\sum_{i=1}^{n} r_{ik}}}$$

$$S_k = \frac{\sum_{i=1}^{n} r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top}{\sum_{i=1}^{n} r_{ik}} = \frac{\sum_{i=1}^{n} r_{ik} \mathbf{x}_i \mathbf{x}_i^\top}{\sum_{i=1}^{n} r_{ik}} - \boldsymbol{\mu}_k \boldsymbol{\mu}_k^\top$$

Just in case

OK if you don't understand

$$\frac{\partial}{\partial \mu_k} = \sum_{i=1}^{n} r_{ik} S_k^{-1}(x_i - \mu_k) = 0$$

$\Downarrow$ multiplying S_k

$$\sum_{i=1}^{n} r_{ik}(x_i - \mu_k) = 0$$

$$\Downarrow \quad \mu_k = \frac{\sum_{i=1}^{n} r_{ik} x_i}{\sum_{i=1}^{n} r_{ik}}$$

$$\frac{\partial}{\partial S_k} = \sum_{i=1}^{n} r_{ik}\left[\frac{1}{2} S_k^{-1} - \frac{1}{2} S_k^{-1}(x_i - \mu_k)(x_i - \mu_k)^T S_k^{-1}\right] = 0$$

$\Downarrow$ multiplying S_k twice

$$\left(\sum_{i=1}^{n} r_{ik}\right) \cdot S_k = \sum_{i=1}^{n} r_{ik}(x_i - \mu_k)(x_i - \mu_k)^T$$

$$\Downarrow \quad S_k = \frac{\sum_{i=1}^{n} r_{ik}(x_i - \mu_k)(x_i - \mu_k)^T}{\sum_{i=1}^{n} r_{ik}}$$

multiplying constant does not change min

adding constant does not change min

$$\min_{\substack{\pi_k \geq 0 \\ \sum_k \pi_k = 1}} \sum_{i=1}^{n}\sum_{k=1}^{K} r_{ik} \log\frac{1}{\pi_k} = \sum_{k=1}^{K} \underbrace{\left(\sum_{i=1}^{n} r_{ik}\right)}_{\text{def } r_k} \log\frac{1}{\pi_k} \equiv \min_{\substack{\pi_k \geq 0 \\ \sum_k \pi_k = 1}} \frac{1}{n}\sum_{k=1}^{K} r_k \log\frac{1}{\pi_k} + \sum_{k=1}^{K} \frac{r_k}{n} \log\frac{r_k}{n}$$

$$= \min_{\substack{\pi_k \geq 0 \\ \sum_k \pi_k = 1}} KL\left(\frac{r}{n} \,\Big\|\, \pi\right) \Rightarrow \pi_k = \frac{r_k}{n}$$

EM for GMM: step 2

$$\pi_k \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_k, S_k)$$

$$\min_{r_{ik} \geq 0, \sum_k r_{ik} = 1} \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left[\sum_{k=1}^{K} r_{ik} \log r_{ik} - \sum_{k=1}^{K} r_{ik} \log p(\mathbf{x}_i, z_i | \boldsymbol{\theta}) \right]$$

$$\boxed{r_{ik} = p(z_i = k | \mathbf{x}_i, \boldsymbol{\theta})} \longrightarrow \text{posterior}$$

$$\propto p(z_i = k) \cdot p(\mathbf{x}_i | z_i = k, \boldsymbol{\theta})$$

prior

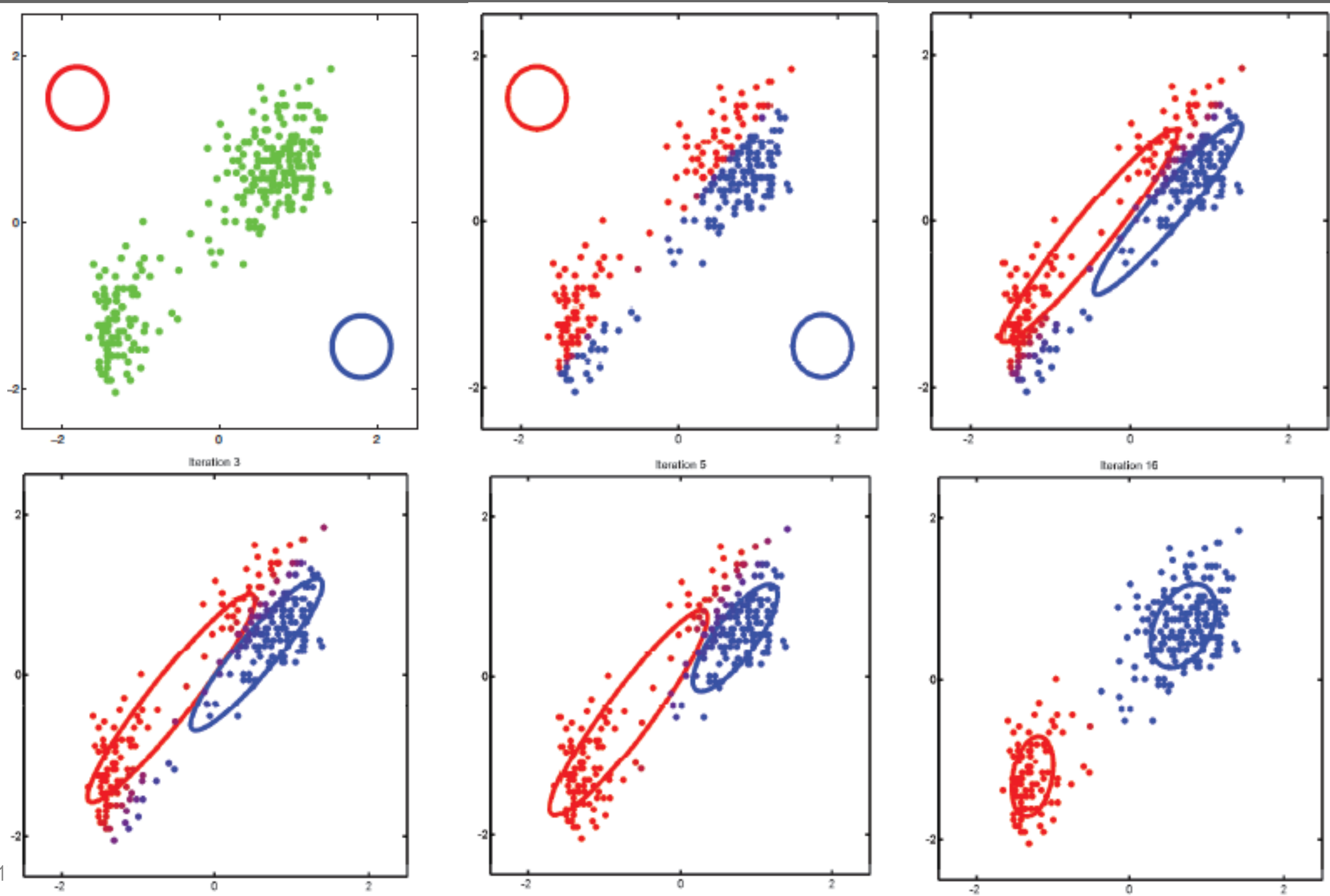
likelihood

$$= \pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, S_k)$$

$$p(z|x) = \frac{p(z,x)}{p(x)} = \frac{p(z) \cdot p(x|z)}{p(x)}$$

$$r_{ik} = \frac{\pi_k |S_k|^{-1/2} \exp(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top S_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k))}{\sum_{c=1}^{K} \pi_c |S_c|^{-1/2} \exp(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_c)^\top S_c^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_c))}$$

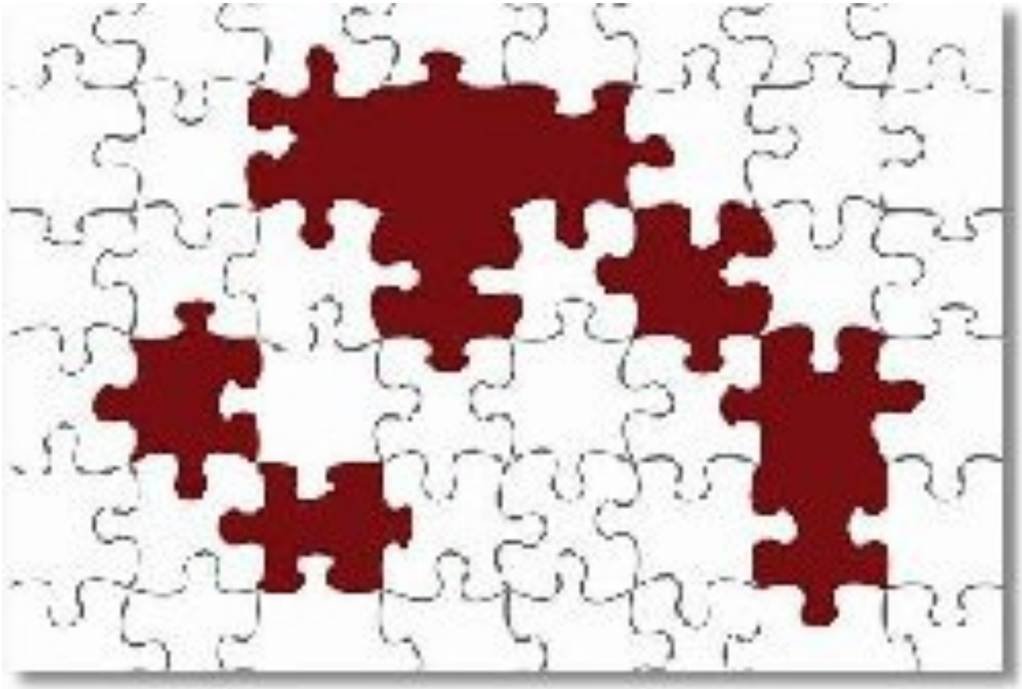
Example



Other uses of EM

- Simplify computation
  - t-distribution as a Gaussian scale-mixture

- Missing data



UNIVERSITY OF WATERLOO

Questions?