# Advanced Machine Learning
# Course V - Mixture Models


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**Option Mathématiques Appliquées**

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# Contents

# Key references for this course

- Bishop, C. M. *Pattern Recognition and Machine Learning.* Springer, 2006.
- Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction.* Second edition. Springer, 2009.
- James, G., Witten, D., Hastie, T. and Tibshirani, R. *An Introduction to Statistical Learning, with Applications in R.* Springer, 2013

Course 5

## Mixture models

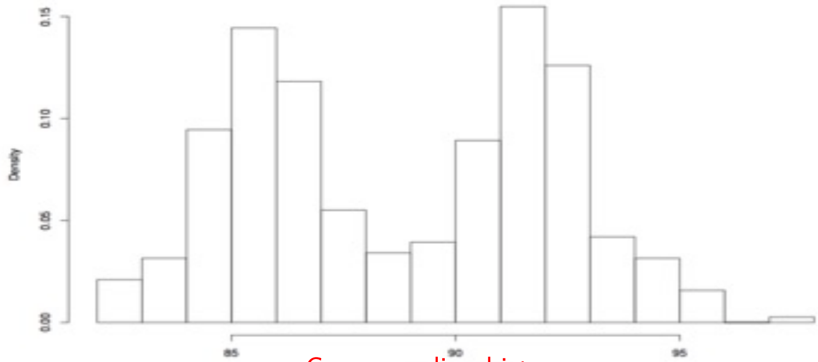
# What it is useful for?

- Data-to-knowledge
  - Statistical models fitting $\Rightarrow$ models learning
  - Features extraction for data, e.g. behavior, shapes...
  - Data characterisation $\Rightarrow$ Complex modelling
- Complex estimation problems, e.g. many parameters, non parametric estimation...
- Clustering / Classification: Modes $\simeq$ clusters / classes
- Dealing with missing (latent) data: unknown labels can be generalized to unobserved data...

# Gaussian Mixture Model

Example: Weight of small animals coming from two different regions

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Length | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 |
| Observations | 5 | 3 | 12 | 36 | 55 | 45 | 21 | 13 |
| Length | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 98 |
| Observations | 15 | 34 | 59 | 48 | 16 | 12 | 6 | 1 |




Corresponding histogram

# Gaussian Mixture Model with two components

To understand / intuite the process, continue with this simple example

$$\begin{aligned} Y_1 &\sim \mathcal{N}(\mu_1, \sigma_1^2) \\ Y_2 &\sim \mathcal{N}(\mu_2, \sigma_2^2) \\ Z &\sim \mathcal{B}(1, p) \end{aligned}$$

That is $P(Z=1) = p$ and $P(Z=0) = 1-p$. In this context, the observations are as follows:

$$X = Z\,Y_1 + (1-Z)\,Y_2$$

**Meanings**

data *follows the first distribution / belongs to the first cluster* with a probability $p$.

Denote $\phi_\theta(x)$ the Gaussian PDF with parameters $\theta = (\mu, \sigma^2)$, one has the following PDF for $X$: $f_X(x) = p\,\phi_{\theta_1}(x) + (1-p)\,\phi_{\theta_2}(x)$ leading to the log-likelihood for $n$ observations $(X_1, \ldots, X_n)$

$$l(\theta; \mathbf{x}) = \sum_{i=1}^{n} \log\left(p\,\phi_{\theta_1}(x_i) + (1-p)\,\phi_{\theta_2}(x_i)\right)$$

# Gaussian Mixture Model with two components

**Difficult estimation problem for $\theta = (p, \theta_1, \theta_2)$, 5 unknown parameters for the simplest case...** Problem with the sum in the log.

Solution: consider unobserved latent variables $(Z_1, \ldots, Z_n)$ where $Z_i = 1$ when $X_i$ comes from the first model and $Z_i = 0$ when $X_i$ comes from the second model. Let us now assume we knew the value of each $Z_i$. In that case, MLEs can be trivially obtained...

$$
\begin{aligned}
l(\theta; \mathbf{x}, \mathbf{z}) = & \sum_{i=1}^{n} \left( z_i \log(\phi_{\theta_1}(x_i)) + (1 - z_i) \log(\phi_{\theta_2}(x_i)) \right) \\
& + \sum_{i=1}^{n} \left( z_i \log(p) + (1 - z_i) \log(1 - p) \right)
\end{aligned}
$$

where $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{z} = (z_1, \ldots, z_n)$.

Derive the MLEs pour $\theta = (p, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$!

# Gaussian Mixture Model with two components

In practice, the values of the $Z_i$'s are **unknown**!

Idea: Replace for each $Z_i$, its expected value (conditional to the observed data $X_i$)

$$\gamma_i(\theta) = E[Z_i|\theta, \mathbf{x}] = P(Z_i = 1|\theta, \mathbf{x})$$

called the responsibility for model 1 of observation $i$. $\Rightarrow$ iterative algorithm, Expectation-Maximization (EM) algo

## Algorithm (EM algo for two-component Gaussian Mixture)

- *Randomly initialization of* $\theta^{(0)}$
- *Repeat until CV for* $t = 0, 1, \ldots$

  (a) ***E-Step:*** *Compute the responsibilities* $\hat{\gamma}_i = \dfrac{\hat{p}\phi_{\hat{\theta}_1}(x_i)}{\hat{p}\phi_{\hat{\theta}_1}(x_i) + (1-\hat{p})\phi_{\hat{\theta}_2}(x_i)}$, $i = 1, \ldots, n$

  (b) ***M-Step:*** *Compute the parameters...* $\hat{\mu}_1 = \dfrac{\sum_i \hat{\gamma}_i x_i}{\sum_i \hat{\gamma}_i}, \hat{\sigma}_1^2 = \dfrac{\sum_i \hat{\gamma}_i (x_i - \hat{\mu}_1)^2}{\sum_i \hat{\gamma}_i}, \ldots$ *and* $\hat{p} = \sum_i \hat{\gamma}_i / n$.

Discussion

# Gaussian Mixture Model

Idea: One aims at modelling the statistical behaviour from several populations, groups or classes...

Notations:

- $n$ observations of i.i.d. random variables/vectors, denoted $(X_1, \ldots, X_n)$
- $K$ different clusters containing $n_k$ observations. Of course, $n = \sum_{k=1}^{K} n_k$
- $p_k$ the probability of belonging to the $k^{th}$ class and $f_k$ the PDF of r.v. in this class.

e.g.,:

- different objects in an image (or a patch) containing $N$ pixels, denoted $x_i$
- population of ducks: $x_i$ corresponds to the size of the $i^{th}$ duck. Different classes corresponding to the animal age/sex/origin (young, old, female, male).
- ...

# Gaussian Mixture Model

Statistical modelling of a mixture: with previous notations, one can defined the following PDF:

$$f(x) = \sum_{k=1}^{K} p_k \times f_k(x)$$

Particular case of Gaussian Mixture Models:

$$f(x) = \sum_{k=1}^{K} p_k \times \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$$

Problem: estimation of many unknown parameters

$$\theta = \left(p_k, \mu_k, \sigma_k\right)_{k=1,\dots,K}$$

with $\sum_{k=1}^{K} p_k = 1$ and $\forall k \in \{1,\dots,K\}, \mu_k \in \mathbb{R}, \sigma_k \in \mathbb{R}_+^*$.

What about $K$ ? Known, unknown ?

# Interest of GMM

GMM allow to model many various distributions

(a) $\frac{1}{5}\mathcal{N}(0,1) + \frac{1}{5}\mathcal{N}(1/2,(2/3)^2) + \frac{3}{5}\mathcal{N}(13/15,(5/9)^2)$,

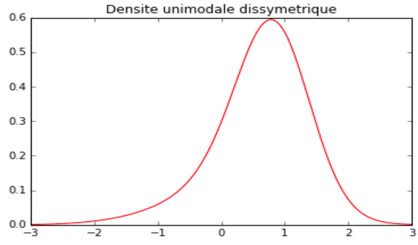
(b) $\sum_{k=0}^{7} \mathcal{N}(3((2/3)^k - 1),(2/3)^{2k})$

(c) $\frac{1}{2}\mathcal{N}(-1,(2/3)^2) + \frac{1}{2}\mathcal{N}(1,(2/3)^2)$

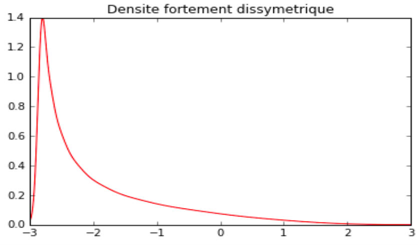
(d) $\frac{3}{4}\mathcal{N}(0,1) + \frac{1}{4}\mathcal{N}(3/2,(1/3)^2)$

(e) $\frac{9}{2}0\mathcal{N}(-6/5,(3/5)^2) + \frac{9}{2}0\mathcal{N}(6/5,(3/5)^2) + \frac{1}{1}0\mathcal{N}(0,(1/4)^2)$

(f) $\frac{1}{2}\mathcal{N}(0,1) + \sum_{k=-2}^{2} \frac{2^{1-k}}{31}\mathcal{N}(k+1/2,(2^{-k}/10)^2)$

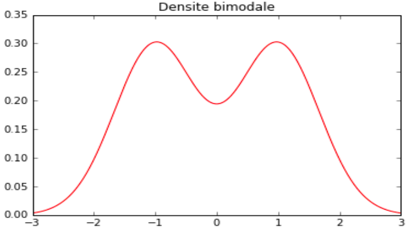



*(a) Asymmetric unimodal PDF*

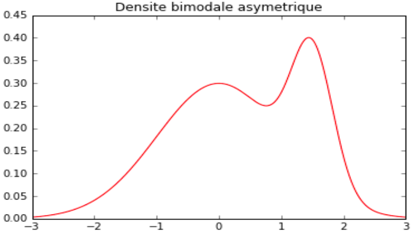



*(b) Strongly asymmetric unimodal PDF*

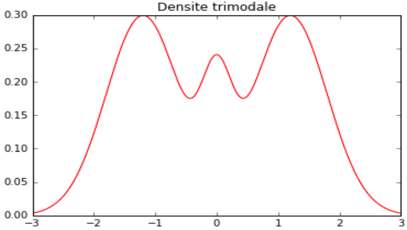
# Interest of GMM



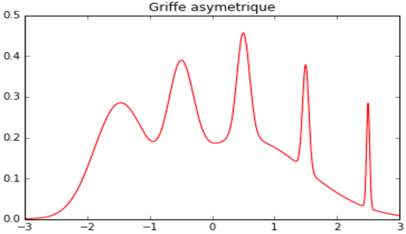

*(c) Bimodal PDF*




*(d) Asymmetric bimodal PDF*




*(e) Tri-modal PDF*




*(f) More complex PDF*

I. Gaussian Mixture Model

II. Reminders in Bayesian probabilities/statistics

III. EM algorithm

IV. Applications

# Reminders in Bayesian probabilities/statistics

For two events (or r. v. ...), one has:

- Conditional probabilities

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

- Bayes rule

$$P(B|A) = \frac{P(A|B)\, P(B)}{P(A)}$$

- if $B_1, \dots, B_n$ is a partition of $\Omega$, i.e. $\bigcup_{i=1}^{n} B_i = \Omega$ and $\forall i \neq j, B_i \cap B_j = \emptyset$, then

$$P(A) = \sum_{i=1}^{n} P(A \cap B_i)$$

# GMM simulations

To simulate the mixture $f(x) = \sum_{k=1}^K p_k \times \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$, one needs to introduce a latent variable $Z$ (or missing data) that corresponds to the class of the variable $X$.

Now, the complete data $T = (X, Z)$ is defined by:

- $Z$ follows a discrete distribution $(p_1, \ldots, p_K)$ on $\{1, \ldots, K\}$ such that $\forall k$, one has (Multinomial distribution)

$$P(Z = k) = p_k, \text{ with } \sum_k p_k = 1$$

- $\forall k \in \{1, \ldots, K\}$, conditionally to $\{Z = k\}$, $X$ has a PDF $f_k$:

$$\mathscr{L}(x|Z = k) = f_k(x)$$

Goal: estimation of $\theta = \left(p_k, \mu_k, \sigma_k\right)_{k=1,\ldots,K}$

2 cases for : one knows latent variables (unrealistic scenario) or not...

# EM algorithm - preliminaries

Simple case: $Z$ is known

$\Rightarrow$ one observes $(x_i, z_i)_{i=1,\dots,n}$ instead of (only) $(x_i)_{i=1,\dots,n}$.
Maximum Likelihood approach

**Theorem (ML estimates of $\theta$)**

*Let the observations $(x_i, z_i)_{i=1,\dots,n}$, then $\forall k \in \{1, \dots, K\}$, one has*

$$\hat{p}_k = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{z_i=k} \tag{1}$$

$$\hat{\mu}_k = \frac{1}{n\,\hat{p}_k}\sum_{i|z_i=k} x_i \tag{2}$$

$$\hat{\sigma}_k^2 = \frac{1}{n\,\hat{p}_k}\sum_{i|z_i=k} (x_i - \hat{\mu}_k)^2 \tag{3}$$

# General EM algorithm - $k$-means, SEM...

General idea: One only observes $(x_1, \ldots, x_n) \Rightarrow$ analyse the log-likelihood

$$l_{obs}(x_1, \ldots, x_n; \theta) = \sum_{i=1}^{n} \log\left(\sum_{k=1}^{K} p_k \times f_k(x_i)\right), \text{ where } \theta = \left(p_k, \mu_k, \sigma_k\right)_{k=1,\ldots,K}$$

Difficult to maximize!!!

BUT one can make assumptions of the unobserved $(Z_1, \ldots, Z_n)$:

**Lemma (Conditional distribution of the $Z_i$'s)**

*For $\theta \in \Theta, x \in \mathbb{R}$ and $k \in \{1, \ldots, K\}$, one has*

$$P_\theta\left(Z = k | X = x\right) = \frac{p_k \times f_k(x)}{\sum_{l=1}^{K} p_l \times f_l(x)} \tag{4}$$

Intuition: thanks to some $\theta_{old}$, one can assign to each $x_i$ some $z_i$ (Lemma) and thanks to previous theorem, one can compute a $\theta_{new}$...

# General EM algorithm - $k$-means, SEM...

Several possible approaches:

- [$k$-means] Assign a class to each $x_i$ according to

$$z_i = \arg\max_k P_{\theta_{old}}(Z = k | X_i = x_i)$$

Natural approach but not flexible

- [SEM] *Randomly* assign a class to each $x_i$ according to the distribution

$$P_{\theta_{old}}(Z = . | X_i = x_i)$$

More flexible

- [$N$-SEM] *Randomly* assign $N$ classes to each $x_i$
- [EM] Limit of $N$-SEM when $N \to \infty$ Very flexible and robust!

# $k$-means

One has to assume that (Very strong assumptions!)

- $p_1 = \ldots = p_K = \dfrac{1}{K}$ and $\sigma_1 = \ldots = \sigma_K$.

## Lemma

$\forall \theta, \forall x \in \mathbb{R}$

$$\mathit{arg}\max_k P_\theta \left(Z = k | X = x\right) = \mathit{arg}\min_k |x - \mu_k|$$

## Algorithm ($k$-means)

- *Randomly initialize* $(z_1, \ldots, z_K)$
- *Repeat until CV:*
  - *for* $k \in \{1, \ldots, K\}$, $\mu_k = \dfrac{1}{n} \sum_{i=1}^{n} x_i \, \mathbb{1}_{z_i = k}$
  - *for* $i \in \{1, \ldots, n\}$, $z_i = \mathit{arg}\min_k |x - \mu_k|$

Advantages / Drawbacks ...

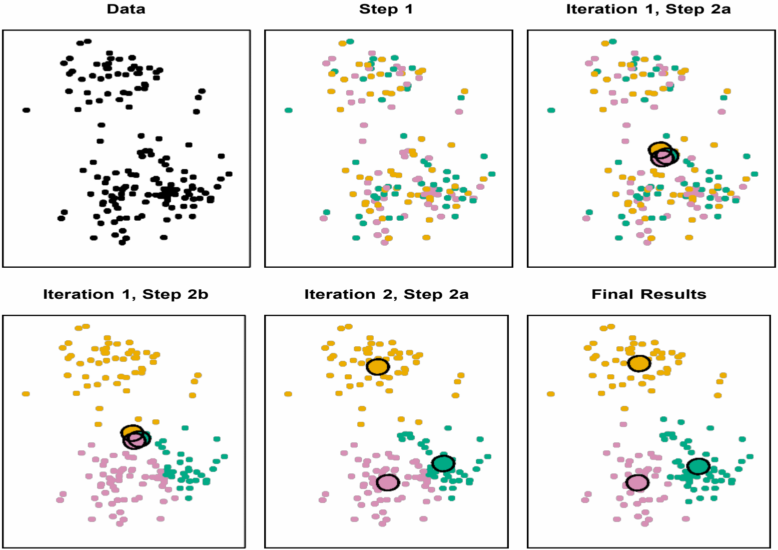
# *Stochastic* EM

General idea: Stochastic version of the $k$-means algorithm...

## Algorithm (SEM)

- *Randomly initialize* $(z_1, \dots, z_K)$
- *Repeat until CV:*
  (a) *Compute*
  $$\hat{\theta} = \arg\max_{\theta} l_{obs}((x_1, z_1), \dots, (x_n, z_n); \theta)$$
  *thanks to Theorem (MLE)*
  (b) *for* $i \in \{1, \dots, n\}$, *randomly choose* $z_i$ *according to*
  $$P_{\hat{\theta}}(Z = .|X_i = x_i)$$
  *given by Eq.* (4).

# *Stochastic* EM



# *Stochastic* EM - $N$ trials

## Algorithm ($N$-SEM (1))

- *Replicate $N$ times, the observations* $(x_1, \ldots, x_n) \to \left(x_i^{(j)}\right)_{1 \le i \le n, 1 \le j \le N}$
- *Apply SEM algo to this dataset.*

## Algorithm ($N$-SEM (2))

- *Randomly initialize $N$ classes* $z_i^1, \ldots, z_i^N \in \{1, \ldots, K\}, \forall i$
- *Repeat until CV*
  (a) *Compute*
  $$\hat{\theta} = \arg\max_{\theta} l_{obs}\left((x_i, z_i^1)_{i=1,\ldots,n} \cup \ldots \cup (x_i, z_i^N)_{i=1,\ldots,n}; \theta\right)$$
  *thanks to Theorem (MLE)*
  (b) *for $i \in \{1, \ldots, n\}$, randomly choose $z_i^1, ..., z_i^N$ (independently!) according to*
  $$P_{\hat{\theta}}\left(Z = .|X_i = x_i\right)$$
  *given by Eq.* (4).

# Expectation-Maximization algorithm

General idea: $N$-SEM with $N \to +\infty$ ...

## Lemma

*Given* $(x_i)_{1\le i\le n}$ *and associated classes for* $N$ *trials* $(z_i^k)_{1\le i\le n, 1\le k\le K}$, *one has*

$$\forall\theta, l_{obs}\left(\left(x_i, z_i^1\right)_{i=1,\dots,n} \cup \dots \cup \left(x_i, z_i^N\right)_{i=1,\dots,n}; \theta\right) = \sum_{j=1}^{N} l_{obs}\left(\left(x_i, z_i^j\right)_{i=1,\dots,n}; \theta\right)$$

## Theorem (First part)

*Given the observations* $(x_i)_{1\le i\le n}$ *and* $\theta_{old} \in \Theta$.

(a) *Let* $Z_1, \dots, Z_n$ *independent r.v. such that* $Z_i \sim \mathcal{L}_{\theta_{old}}(Z|X = x_i)$. *One has* $\forall\theta = (p_k, \mu_k, \sigma_k)_{1\le k\le K} \in \Theta$,

$$E[l\left((x_i, z_i)_{i=1,\dots,n}; \theta\right)] = \sum_{i=1}^{n}\sum_{k=1}^{K} P_{\theta_{old}}(Z = k|X = x_i) \log\left(p_k \times f_k(x_i)\right)$$

*where* $P_{\theta_{old}}(Z = .|X = x_i)$ *given by Eq.* (4).

# Expectation-Maximization algorithm

## Theorem (Second part)

*Given the observations* $(x_i)_{1\le i\le n}$ *and* $\theta_{old}\in\Theta$,

(b) *One has that* $\underset{\theta}{\operatorname{argmax}} E[l((x_i,z_i)_{i=1,\dots,n};\theta)]$ *is given by:*

- ***Classes probabilities:*** $\forall k=1,\dots,K$,

$$p_k^{argmax}=\frac{1}{n}\sum_{i=1}^{n}P_{\theta_{old}}(Z=k|X=x_i)$$

- ***Classes means:*** $\forall k=1,\dots,K$,

$$\mu_k^{argmax}=\frac{1}{n\,p_k^{argmax}}\sum_{i=1}^{n}P_{\theta_{old}}(Z=k|X=x_i)\;x_i$$

- ***Classes variances:*** $\forall k=1,\dots,K$,

$$(\sigma_k^{argmax})^2=\frac{1}{n\,p_k^{argmax}}\sum_{i=1}^{n}P_{\theta_{old}}(Z=k|X=x_i)\;(x_i-\mu_k^{argmax})^2$$

# Expectation-Maximization algorithm

Following previous theorem, one has the following theoretical algorithm:

**Algorithm (Theory)**

- *Randomly initialization of* $\theta_0$
- *Repeat until CV for* $t = 0, 1, \ldots$

  (a) ***E-Step:*** *Compute*

  $$L_t(\theta) = E\left[ l\left( \left(X_i, Z_i^t\right)_{i=1,\ldots,n}; \theta \right) \right] \left( \Longleftrightarrow Q(\theta, \theta_t) = E\left( l(\theta; \mathbf{t}) | \mathbf{x}, \theta_t \right) \right)$$

  *where* $Z_1^t, \ldots, Z_n^t$ *are i.i.d. with* $Z_i^t \sim \mathcal{L}_{\theta_t}(Z|X = x_i)$

  (b) ***M-Step:*** *Maximize* $L_t(\theta)$ *to obtain* $\theta_{t+1} = \text{arg}\max_\theta L_t(\theta)$

- **E** for *Expectation*
- **M** for *Maximization*

Outline of the proof...

# Expectation-Maximization algorithm

In practice, one has to implement the following algorithm...

## Algorithm (Practice)

- *Randomly initialization of* $\theta_0$
- *Repeat until CV for* $t = 0, 1, \ldots$
  (a) ***E-Step:*** *Compute the matrix*

$$\left[P_{\theta_t}(Z = k|X = x_i)\right]_{1 \le i \le n, 1 \le k \le K} = \left[\frac{p_k^t \times f_{k,t}(x_i)}{\sum_{l=1}^K p_l^t \times f_{l,t}(x_i)}\right]_{1 \le i \le n, 1 \le k \le K}$$

  (b) ***M-Step:*** *Compute* $\theta_{t+1}$, *for all* $k = 1, \ldots, K$,

$$\hat{p}_k^{t+1} = \frac{1}{n}\sum_{i=1}^n P_{\theta_t}(Z = k|X = x_i), \quad (5)$$

$$\hat{\mu}_k^{t+1} = \frac{1}{n\hat{p}_k^{t+1}}\sum_{i=1}^n x_i P_{\theta_t}(Z = k|X = x_i) \quad (6)$$

$$\left(\hat{\sigma}_k^{t+1}\right)^2 = \frac{1}{n\hat{p}_k^{t+1}}\sum_{i=1}^n P_{\theta_t}(Z = k|X = x_i)\left(x_i - \hat{\mu}_k^{t+1}\right)^2 \quad (7)$$

# A different view - *Maximization-Maximization* procedure

- Consider the function $F(\theta,\mathbf{P}) = E_{\mathbf{P}}[l_0(\theta;\mathbf{t})] - E_{\mathbf{P}}[\log(\mathbf{P}(\mathbf{z}))]$
- $\mathbf{P}$ can be any distribution for the *latent* variables $\mathbf{z}$.
- Note that $F$ evaluated at $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x},\theta)$ is the log-likelihood of the observed data.
- EM algo can be viewed as a joint maximization method for $F$ over $\theta$ and $\mathbf{P}(\mathbf{z})$. Maximizer over $\mathbf{P}(\mathbf{z})$ for fixed $\theta$ can be shown to be $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x},\theta)$. (dist. computed at the $E$-step).
- $M$-step: Maximize $F(\theta,\mathbf{P})$ over $\theta$ for fixed $\mathbf{P}(\mathbf{z})$, $\Longleftrightarrow$ maximizing $E_{\mathbf{P}}[l_0(\theta;\mathbf{t})|\mathbf{x},\theta^*]$ (2nd term do not depend on $\theta$).

Since $F(\theta,\mathbf{P})$ and the obs. data log-likelihood agree when $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x},\theta)$, maximization of the former accomplishes maximization of the latter.

# Applications to image processing with Mixtures of Asymmetric Generalized Gaussian distributions

Course 5

New slides