#### **Bayesian Models in Machine Learning**

GMM, EM algorithm

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- or ...

## Multivariate GMM - recapitulation



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- or ...

# BN for GMM – recapitulation

$$p(x) = \sum_{z} p(x|z)P(z) = \sum_{c} \mathcal{N}(x; \mu_{c}, \sigma_{c}^{2})\operatorname{Cat}(z = c|\boldsymbol{\pi})$$

 or we can see it as a generative probabilistic model described by Bayesian network with Categorical latent random variable z identifying Gaussian distribution generating the observation x

$$\begin{array}{c} z \\ p(x,z) = p(x|z)P(z) \\ x \end{array}$$

- Observations are assumed to be generated as follows:
  - randomly select Gaussian component according probabilities P(z)
  - generate observation *x* form the selected Gaussian distribution
- To evaluate p(x), we have to marginalize out z
- No close form solution for training

# BN for GMM – recapitulation II

• Multiple observations:



$$p(x_1, x_2, ..., x_N, z_1, z_2, ..., z_N) = \prod_{n=1}^N p(x_n | z_n) P(z_n)$$

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- Re-estimate parameters of Gaussians using the data assigned to them in the previous step.
   New weights will be proportional to the number of data points assigned to the Gaussians.



- Intuitive and Approximate iterative algorithm for training GMM parameters.
- Using current model parameters, let Gaussians classify data as if the Gaussians were different classes (Even though all the data corresponds to only one class modeled by the GMM)
- Re-estimate parameters of Gaussians using the data assigned to them in the previous step.
   New weights will be proportional to the number of data points assigned to the Gaussians.
- Repeat the previous two steps until the algorithm converges.



# Training GMM – EM algorithm

- **Expectation Maximization** is a general tool applicable to different generative models with latent (hidden) variables.
- Here, we only see the result of its application to the problem of re-estimating GMM parameters.
- It guarantees to increase the likelihood of training data in every iteration. However, it does not guarantee to find the global optimum.
- The algorithm is very similar to the Viterbi training presented above. However, instead of hard alignments of observations to Gaussian components, the posterior probabilities  $P(c|x_i)$  (calculated given the old model) are used as soft weights. Parameters  $\mu_c, \sigma_c^2$  are then calculated using a weighted average.

$$\gamma_{nc} = \frac{\mathcal{N}\left(x_{n} | \mu_{c}^{(old)}, \sigma_{c}^{2} \right) \pi_{c}^{(old)}}{\sum_{k} \mathcal{N}\left(x_{n} | \mu_{k}^{(old)}, \sigma_{k}^{2} \right) \pi_{k}^{(old)}} = \frac{p(x_{n} | z_{n} = c) P(z_{n} = c)}{\sum_{k} p(x_{n} | z_{n} = k) P(z_{n} = k)} = P(z_{n} = c | x_{n})$$

$$\mu_c^{(new)} = \frac{1}{\sum_n \gamma_{nc}} \sum_n \gamma_{nc} \mathbf{x}_n$$

$$\pi_c^{(new)} = \frac{\sum_n \gamma_{nc}}{\sum_k \sum_n \gamma_{nc}} = \frac{\sum_n \gamma_{nc}}{N}$$

$$\sigma_{c}^{2(new)} = \frac{1}{\sum_{n} \gamma_{nc}} \sum_{n} \gamma_{nc} \left( \mathbf{x}_{n} - \mu_{c}^{(new)} \right)^{2}$$

## GMM to be learned











![](_page_15_Figure_1.jpeg)

## Expectation maximization algorithm

![](_page_16_Figure_1.jpeg)

- where  $q(\mathbf{Z})$  is any distribution over the latent variable
- Kullback-Leibler divergence  $D_{KL}(q||p)$  measures "unsimilarity" between two distributions q, p
- $D_{KL}(q||p) \ge 0$  and  $D_{KL}(q||p) = 0 \Leftrightarrow q = p$
- $\Rightarrow$  Evidence lower bound (ELBO)  $\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta}) \leq p(\mathbf{X}|\boldsymbol{\eta})$
- $H(q(\mathbf{Z}))$  is (non-negative) Entropy of distribution  $q(\mathbf{Z})$
- $Q(q(\mathbf{Z}), \boldsymbol{\eta})$  is called auxiliary function.

## Expectation maximization algorithm

 $\ln p(\mathbf{X}|\boldsymbol{\eta}) = \underbrace{\mathcal{Q}(q(\mathbf{Z}),\boldsymbol{\eta}) + H(q(\mathbf{Z}))}_{\mathcal{L}(q(\mathbf{Z}),\boldsymbol{\eta})} + D_{KL}\left(q(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X},\boldsymbol{\eta})\right)$ 

• We aim to find parameters  $\boldsymbol{\eta}$  that maximize  $\ln p(\mathbf{X}|\boldsymbol{\eta})$ 

• E-step: 
$$q(\mathbf{Z}) \coloneqq P(\mathbf{Z}|\mathbf{X}, \boldsymbol{\eta}^{old})$$

- makes the  $D_{KL}(q||p)$  term 0
- makes  $\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta}) = \ln p(\mathbf{X}|\boldsymbol{\eta})$
- M-step:  $\eta^{new} = \underset{\eta}{\arg \max} Q(q(\mathbf{Z}), \eta)$ 
  - $D_{KL}(q||p)$  increases as  $P(\mathbf{X}|\mathbf{Z}, \boldsymbol{\eta})$  deviates from  $q(\mathbf{Z})$
  - $H(q(\mathbf{Z}))$  does not change for fixed  $q(\mathbf{Z})$
  - $\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta})$  increases like  $\mathcal{Q}(q(\mathbf{Z}), \boldsymbol{\eta})$
  - $\ln p(\mathbf{X}|\boldsymbol{\eta})$  increases more than  $Q(q(\mathbf{Z}), \boldsymbol{\eta})$

![](_page_18_Figure_0.jpeg)

## Expectation maximization algorithm

 $Q(q(\mathbf{Z}), \boldsymbol{\eta})$  and  $\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta})$  will be easy to optimize (e.g. quadratic function) compared to  $\ln p(\mathbf{X}|\boldsymbol{\eta})$ 

![](_page_19_Figure_2.jpeg)

# EM for GMM

• Now, we aim to train parameters  $\eta = \{\mu_z, \sigma_z^2, \pi_z\}$  of Gaussian Mixture model

$$p(x) = \sum_{z} p(x|z)P(z) = \sum_{c} \mathcal{N}(x; \mu_{c}, \sigma_{c}^{2})\operatorname{Cat}(z = c|\boldsymbol{\pi})$$

• Given training observations  $\mathbf{x} = [x_1, x_2, ..., x_N]$  we search for ML estimate of  $\boldsymbol{\eta}$  that maximizes log likelihood of the training data.

$$\ln p(\mathbf{x}) = \sum_{n} \ln p(x_n) = \sum_{n} \left[ \ln \sum_{c} \mathcal{N}(x_n; \mu_c, \sigma_c^2) - \pi_c \right]$$

- Direct maximization of this objective function w.r.t.  $\eta$  is intractable.
- We will use EM algorithm, where we maximize the auxiliary function which is (for simplicity) sum of per-observation auxiliary functions

$$Q(q(\mathbf{z}), \boldsymbol{\eta}) = \sum_{n} Q_n(q(z_n), \boldsymbol{\eta})$$

• Again, in M-step  $\sum_{n} \ln p(x_n)$  has to increase more than  $\sum_{n} Q_n(q(z_n), \eta)$ 

# EM for GMM – E-step

$$q(z_n) = P(z_n | x_n, \boldsymbol{\eta}^{old})$$
$$= \frac{p(x_n | z_n, \boldsymbol{\eta}^{old}) P(z_n | \boldsymbol{\eta}^{old})}{p(x_n | \boldsymbol{\eta}^{old})}$$

$$q(z_n = c) = \frac{\mathcal{N}(x_n | \mu_c^{old} \sigma_c^{2^{old}}) \pi_c^{old}}{\sum_k \mathcal{N}(x_n | \mu_k^{old}, \sigma_k^{2^{old}}) \pi_k^{old}} = \gamma_{nc}$$

- γ<sub>nc</sub> is the so called responsibility of Gaussian component z for observation n.
- It is the probability for an observation n being generated from component c

## EM for GMM – M-step

$$Q(q(\mathbf{z}), \boldsymbol{\eta}) = \sum_{n} Q_{n}(q(z_{n}), \boldsymbol{\eta})$$
$$= \sum_{n} \sum_{z_{n}} q(z_{n}) \ln p(x_{n}, z_{n} | \boldsymbol{\eta})$$
$$= \sum_{n} \sum_{c} \gamma_{nc} \left[ \ln \mathcal{N}(x_{n}; \mu_{c}, \sigma_{c}) + \ln \pi_{c} \right]$$

• In M-step, the auxiliary function is maximized w.r.t. all GMM parameters

# EM for GMM –update of means

• Update for component mean means:

$$\frac{\partial}{\partial \mu_c} \sum_n Q_n(q(z_n), \eta) = \frac{\partial}{\partial \mu_c} \sum_n \sum_k \gamma_{nk} \left[ \ln \mathcal{N}(x_n; \mu_k, \sigma_k^2) + \ln \pi_k \right]$$
$$= \frac{\partial}{\partial \mu_c} \sum_n \gamma_{nc} \left[ -\frac{(x_n - \mu_c)^2}{2\sigma_c^2} + K \right]$$
$$= \frac{1}{\sigma_c^2} \sum_n \gamma_{nc}(\mu_c - x_n) = 0$$
$$\Longrightarrow \mu_c = \frac{\sum_n \gamma_{nc} x_n}{\sum_n \gamma_{nc}}$$

• Update for variances:  $\sigma_c^2 = \frac{\sum_n \gamma_{nc} (x_n - \mu_c)^2}{\sum_n \gamma_{nc}}$  can be derived similarly.

#### Flashback: ML estimate for Gaussian

$$\arg\max_{\mu,\sigma^2} p(\mathbf{x}|\mu,\sigma^2) = \arg\max_{\mu,\sigma^2} \ln p(\mathbf{x}|\mu,\sigma^2) = \sum_i \ln \mathcal{N}(x_n;\mu,\sigma^2)$$
$$= -\frac{1}{2\sigma^2} \sum_n x_n^2 + \frac{\mu}{\sigma^2} \sum_n x_n - N \frac{\mu^2}{2\sigma^2} - \frac{\ln(2\pi)}{2}$$

$$\frac{\partial}{\partial \mu} \ln p(\mathbf{x}|\mu, \sigma^2) = \frac{\partial}{\partial \mu} \left( -\frac{1}{2\sigma^2} \sum_n x_n^2 + \frac{\mu}{\sigma^2} \sum_n x_n - N \frac{\mu^2}{2\sigma^2} - \frac{\ln(2\pi)}{2} \right)$$
$$= \frac{1}{\sigma^2} \left( \sum_n x_n - N \mu \right) = 0 \quad \Rightarrow \quad \hat{\mu}^{ML} = \frac{1}{N} \sum_n x_n$$

and similarly:  $\widehat{\sigma^2}^{ML} = \frac{1}{N} \sum_n (x_n - \mu)^2$ 

# EM for GMM –update of weights

• Weights  $\pi_c$  need to sum up to one. When updating weights, Lagrange multiplier  $\lambda$  is used to enforce this constraint.

$$\frac{\partial}{\partial \pi_c} \left( \sum_n Q_n(q(z_n), \eta) - \lambda \left( \sum_k \pi_k - 1 \right) \right) = \frac{\partial}{\partial \pi_c} \left( \sum_n \sum_k \gamma_{nk} \ln \pi_k - \lambda \left( \sum_k \pi_k - 1 \right) \right) = \sum_n \frac{\gamma_{nc}}{\pi_c} - \lambda = 0$$
$$\Longrightarrow \pi_c = \frac{\sum_n \gamma_{nc}}{\lambda} = \frac{\sum_n \gamma_{nc}}{\sum_k \sum_n \gamma_{nk}}$$

# Factorization of the auxiliary function more formally

• Before, we have introduced the per-observation auxiliary functions

$$Q(q(\mathbf{z}), \boldsymbol{\eta}) = \sum_{n} Q_{n}(q(z_{n}), \boldsymbol{\eta})$$
$$= \sum_{n} \sum_{z_{n}} q(z_{n}) \ln p(x_{n}, z_{n} | \boldsymbol{\eta})$$

• We can show that such factorization comes naturally even if we directly write the auxiliary function as defined for the EM algorithm:

$$Q(q(\mathbf{z}), \boldsymbol{\eta}) = \sum_{\mathbf{z}} q(\mathbf{z}) \ln p(\mathbf{x}, \mathbf{z} | \boldsymbol{\eta}) = \sum_{\mathbf{z}} \prod_{n'} q(z_{n'}) \sum_{n} \ln p(x_n, z_n | \boldsymbol{\eta})$$
$$= \sum_{c} \sum_{n} q(z_n = c) \ln p(x_n, z_n = c | \boldsymbol{\eta})$$

• See the next slide for proof

#### Factorization over components

Example with only 3 observations (i.e.,  $\mathbf{z} = [z_1, z_2, z_3]$ )

$$\sum_{\mathbf{Z}} q(\mathbf{z}) \ln p(\mathbf{x}, \mathbf{z} | \boldsymbol{\eta}) = \sum_{\mathbf{Z}} \prod_{n'} q(z_{n'}) \sum_{n} \log p(x_{n}, z_{n} | \boldsymbol{\eta}) = \sum_{\mathbf{Z}} \prod_{n'} q(z_{n'}) \sum_{n} f(z_{n}) = \sum_{n} \sum_{\mathbf{Z}} \prod_{n'} q(z_{n'}) f(z_{n}) = \sum_{n} \sum_{\mathbf{Z}} \prod_{n'} q(z_{n'}) f(z_{n}) = \sum_{n} \sum_{\mathbf{Z}} \sum_{n'} q(z_{n'}) f(z_{n'}) = \sum_{n} \sum_{\mathbf{Z}} \sum_{n'} q(z_{n'}) f(z_{n'}) + \sum_{n} \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) = \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) + \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) + \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) = \sum_{\mathbf{Z}} \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) + \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) f(z_{n'}) f(z_{n'}) f(z_{n'}) = \sum_{\mathbf{Z}} q(z_{n'}) f(z_{n'}) f(z$$

$$\sum_{c=1}^{C} q(z_1 = c)f(z_1 = c) + \sum_{c=1}^{C} q(z_2 = c)f(z_2 = c) + \sum_{c=1}^{C} q(z_3 = c)f(z_3 = c) =$$

$$\sum_{c=1}^{C} \sum_{n} q(z_n = c) f(z_n = c) = \sum_{c=1}^{C} \sum_{n} q(z_n = c) \log p(x_n, z_n = c | \eta)$$

#### Flashback: Example: BP for HMM

• To evaluation an HMM, given a sequence of observations  $X = [x_1, x_2 \dots, x_N]$ , we need to infer

$$p(\mathbf{X}) = p(x_1, x_2, \dots, x_N) = \sum_{z_1} \sum_{z_2} \dots \sum_{z_N} p(x_1, x_2, \dots, x_N, z_1, z_2, \dots, z_N)$$

• To train an HMM using an EM algorithm (see next lesson), for every t = 1..N, we need to infer

$$p(z_t | \mathbf{X}) = \frac{p(z_t, \mathbf{X})}{p(\mathbf{X})} = \frac{\sum_{z_1} \sum_{z_2} \dots \sum_{z_{t-1}} \sum_{z_{t+1}} \dots \sum_{z_N} p(x_1, x_2 \dots, x_N, z_1, z_2 \dots, z_N)}{p(\mathbf{X})}$$

![](_page_28_Figure_5.jpeg)

![](_page_28_Figure_6.jpeg)

s are state ids (i.e., possible values of  $z_t$ )

$$\alpha(t,s) = p(\mathbf{x}_t|s) \sum_{s'} \alpha(t-1,s')p(s|s')$$
$$\beta(t,s) = \sum_{s'} \beta(t+1,s')p(\mathbf{x}_{t+1}|s')p(s'|s)$$
$$p(\mathbf{X}) = \sum_{s' \in FinalStates} \alpha(N,s')$$
$$p(z_t = s|\mathbf{X}) = \frac{\alpha(t,s)\beta(t,s)}{P(\mathbf{X})}$$

#### Examples: Training HMMs using EM

![](_page_29_Figure_1.jpeg)

E-step:

$$\alpha(t,s) = p(\mathbf{x}_t|s) \sum_{s'} \alpha(t-1,s')p(s|s')$$
$$\beta(t,s) = \sum_{s'} \beta(t+1,s')p(\mathbf{x}_{t+1}|s')p(s'|s)$$

$$\gamma_s(t) = p(z_t = s | \mathbf{X}) = \frac{\alpha(t, s)\beta(t, s)}{\sum_{s' \in Final States} \alpha(N, s')}$$

M-step:

$$\hat{\mu}_s^{(new)} = \frac{\sum_{t=1}^T \gamma_s(t) x(t)}{\sum_{t=1}^T \gamma_s(t)}$$
$$\hat{\sigma}_s^{2(new)} = \frac{\sum_{t=1}^T \gamma_s(t) (x(t) - \hat{\mu}_s^{(new)})^2}{\sum_{t=1}^T \gamma_s(t)}$$

#### EM for continuous latent variable

 Same equations, where sums over the latent variable Z are simply replaced by integrals

$$\ln p(\mathbf{X}|\boldsymbol{\eta}) = \underbrace{\int q(\mathbf{Z}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\eta}) \, \mathrm{d}\mathbf{Z}}_{\mathcal{Q}(q(\mathbf{Z}), \boldsymbol{\eta})} \underbrace{\int q(\mathbf{Z}) \ln q(\mathbf{Z}) \, \mathrm{d}\mathbf{Z}}_{H(q(\mathbf{Z}))} \underbrace{\int q(\mathbf{Z}) \ln \frac{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\eta})}{q(\mathbf{Z})} \, \mathrm{d}\mathbf{Z}}_{D_{KL}(q(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\eta}))}$$

$$= \underbrace{\mathcal{Q}(q(\mathbf{Z}), \boldsymbol{\eta}) + H(q(\mathbf{Z}))}_{\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta})} + D_{KL}\left(q(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\eta})\right)$$

#### Flashback: PLDA model for speaker verification

- Let each speech utterance be represented by *speaker embedding vector* **x** 
  - e.g. 512 dim. output of hidden layer of neural network trained for speaker classification
- We assume, that the distribution of the embeddings can be modeled as follows:
- We assume the same factorization as for GMM, but with continuous laten variable z

 $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}_{ac})$  $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{z}, \boldsymbol{\Sigma}_{wc})$ 

- distribution of speaker means
- within class (channel) variability

 $\mathbf{Z}_{S}$ 

- Observations (embeddings) are assumed to be generated as follows:
  - Latent (speaker mean) vector  $\mathbf{z}_s$  is generated for each speaker s from gaussian distribution  $p(\mathbf{z})$
  - All embeddings of speaker s are generated from Gaussian distribution  $p(\mathbf{x}_{si}|\mathbf{z}_{s})$

![](_page_31_Figure_11.jpeg)