Bayesian Models in Machine Learning

GMM, EM algorithm

Lukáš Burget

BRNO FACULTY UNIVERSITY OF INFORMATION OF TECHNOLOGY TECHNOLOGY

BAYa lectures, October 2023

- We can see the sum above just as a function defining the shape of the probability density function
- $or \dots$

Multivariate GMM - recapitulation

- We can see the sum above just as a function defining the shape of the probability density function
- or \dots

BN for GMM – recapitulation

$$
p(x) = \sum_{z} p(x|z)P(z) = \sum_{c} \mathcal{N}(x; \mu_c, \sigma_c^2) \text{Cat}(z = c | \boldsymbol{\pi})
$$

• 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

$$
\bigcirc^2 z
$$

$$
p(x, z) = p(x|z)P(z)
$$

$$
x
$$

- 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:

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

• Intuitive and Approximate iterative algorithm for training GMM parameters.

- 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)

- 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.

- 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 μ_c , σ_c^2 are then calculated using a weighted average.

$$
\gamma_{nc} = \frac{\mathcal{N}\left(x_n|\mu_c^{(old)}, \sigma^2_c^{(old)}\right)\pi_c^{(old)}}{\sum_k \mathcal{N}\left(x_n|\mu_k^{(old)}, \sigma^2_k^{(old)}\right)\pi_k^{(old)}} = \frac{p(x_n|z_n = c)P(z_n = c)}{\sum_k p(x_n|z_n = k)P(z_n = k)} = P(z_n = c|x_n)
$$

$$
\mu_c^{(new)} = \frac{1}{\sum_n \gamma_{nc}} \sum_n \gamma_{nc} x_n
$$

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

$$
\sigma^2{}_{c}^{(new)} = \frac{1}{\sum_n \gamma_{nc}} \sum_n \gamma_{nc} \left(x_n - \mu_c^{(new)}\right)^2
$$

GMM to be learned

Expectation maximization algorithm

- 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

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

• We aim to find parameters η that maximize $\ln p(X|\eta)$

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

- makes the $D_{\text{KL}}(q || p)$ term 0
- makes $\mathcal{L}(q(\mathbf{Z}), \boldsymbol{\eta}) = \ln p(\mathbf{X}|\boldsymbol{\eta})$
- M-step: $\eta^{new} = \arg \max Q(q(\mathbf{Z}), \eta)$ η
	- $D_{KL}(q||p)$ increases as $P(X|Z, \eta)$ deviates from $q(Z)$
	- $H(q(\mathbf{Z}))$ 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 $Q(q(\mathbf{Z}), \boldsymbol{\eta})$

Expectation maximization algorithm

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

EM for GMM

• Now, we aim to train parameters $\boldsymbol{\eta} = \{\mu_{z}, \sigma_{z}^{2}, \pi_{z}\}$ of Gaussian Mixture model

$$
p(x) = \sum_{z} p(x|z)P(z) = \sum_{c} \mathcal{N}(x; \mu_c, \sigma_c^2) \text{Cat}(z = c | \boldsymbol{\pi})
$$

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

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

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

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

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

EM for GMM – E-step

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

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

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

- γ_{nc} 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

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

=
$$
\sum_{n} \sum_{z_n} q(z_n) \ln p(x_n, z_n | \boldsymbol{\eta})
$$

=
$$
\sum_{n} \sum_{c} \gamma_{nc} [\ln \mathcal{N}(x_n; \mu_c, \sigma_c) + \ln \pi_c]
$$

• 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:

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

$$
= \frac{\partial}{\partial \mu_c} \sum_n \gamma_{nc} \left[-\frac{(x_n - \mu_c)^2}{2\sigma_c^2} + K \right]
$$

$$
= \frac{1}{\sigma_c^2} \sum_n \gamma_{nc} (\mu_c - x_n) = 0
$$

$$
\implies \mu_c = \frac{\sum_n \gamma_{nc} x_n}{\sum_n \gamma_{nc}}
$$

• Update for variances: $\sigma_c^2 = \frac{\sum n \ln c \sqrt{n} m^2}{\sum n}$ can be derived similarly. $\sum_n \gamma_{nc} (x_n - \mu_c)^2$ Σ_n γ $_{nc}$

Flashback: ML estimate for Gaussian

$$
\arg \max_{\mu, \sigma^2} p(\mathbf{x} | \mu, \sigma^2) = \arg \max_{\mu, \sigma^2} \ln p(\mathbf{x} | \mu, \sigma^2) = \sum_{i} \ln \mathcal{N}(x_n; \mu, \sigma^2)
$$

$$
= -\frac{1}{2\sigma^2} \sum_{n} x_n^2 + \frac{\mu}{\sigma^2} \sum_{n} x_n - N \frac{\mu^2}{2\sigma^2} - \frac{\ln(2\pi)}{2}
$$

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

$$
= \frac{1}{\sigma^2} \left(\sum_n x_n - N\mu \right) = 0 \implies \hat{\mu}^{ML} = \frac{1}{N} \sum_n x_n
$$

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

EM for GMM –update of weights

• Weights π_c need to sum up to one. When updating weights, Lagrange multiplier λ is used to enforce this constraint.

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

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., $z = [z_1, z_2, z_3]$)

$$
\sum_{\mathbf{z}} q(\mathbf{z}) \ln p(\mathbf{x}, \mathbf{z} | \mathbf{\eta}) = \sum_{\mathbf{z}} \prod_{n'} q(z_{n'}) \sum_{n} \log p(x_{n}, z_{n} | \mathbf{\eta}) = \sum_{\mathbf{z}} \prod_{n'} q(z_{n'}) \sum_{n} f(z_{n}) = \sum_{n} \sum_{\mathbf{z}} \prod_{n'} q(z_{n'}) f(z_{n}) =
$$
\n
$$
\sum_{z_1} \sum_{z_2} \sum_{z_3} q(z_1) q(z_2) q(z_3) f(z_1) + \sum_{z_1} \sum_{z_2} \sum_{z_3} q(z_1) q(z_2) q(z_3) f(z_2) + \sum_{z_1} \sum_{z_2} \sum_{z_3} q(z_1) q(z_2) q(z_3) f(z_3) =
$$
\n
$$
\sum_{z_1} q(z_1) f(z_1) \sum_{z_2} q(z_2) \sum_{z_3} q(z_3) + \sum_{z_1} q(z_1) \sum_{z_2} q(z_2) f(z_2) \sum_{z_3} q(z_3) + \sum_{z_1} q(z_1) \sum_{z_2} q(z_2) \sum_{z_3} q(z_3) f(z_3) =
$$
\n
$$
\sum_{z_1} q(z_1) f(z_1) + \sum_{z_2} q(z_2) f(z_2) + \sum_{z_3} q(z_3) f(z_3) =
$$

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

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

Flashback: Example: BP for HMM

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

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

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

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

Forward-backward algorithm s are state ids (i.e., possible values of z_t) $\alpha(t,s) = p(\mathbf{x}_t|s)$ $\overline{s'}$ $\alpha(t-1,s')p(s|s')$ $\beta(t, s) = \sum$ $\overline{s'}$ $\beta(t + 1, s')p(\mathbf{x}_{t+1} | s')p(s' | s)$ $p(X) =$ s'∈FinalStates $\alpha(N, s')$ $p(z_t = s | \boldsymbol{X}) =$ $\alpha(t, s) \beta(t, s)$ $P(X)$

Examples: Training HMMs using EM

E-step:

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

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

$$
\gamma_{S}(t) = p(z_t = s | \mathbf{X}) = \frac{\alpha(t, s)\beta(t, s)}{\sum_{s' \in FinalStates} \alpha(N, s')}
$$

M-step:

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

EM for continuous latent variable

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

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

Flashback: PLDA model for speaker verification

- Let each speech utterance be represented by *speaker embedding vector*
	- 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

- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}_{ac})$ distribution of speaker means
- $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{z}, \mathbf{\Sigma}_{wc})$ within class (channel) variability

 $\mathbf{Z}_{\mathcal{S}}$

 X_{Si}

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

