

Mathematics for Machine Learning

— Expectation Maximization

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

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Credits for the resource

- The slides are based on the textbooks:
 - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
 - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

Outline

- 1 Expectation Maximization (EM) Algorithm
- 2 Latent-Variable Perspective

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Motivation

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 - ∵ the complex dependency on the parameters.
- The likelihood approach suggests a simple iterative scheme for finding a solution to the parameters estimation problem.

Expectation Maximization

- A general iterative scheme for learning parameters (MLE or MAP) in mixture models and latent-variable models.

Dempster et al. (1977)

Choose initial parameter values (i.e., μ_k, Σ_k, π_k) and **alternate** between the following two steps until convergence:

- **E-step:** Evaluate the responsibilities r_{ik}
 - It can be viewed as the **posterior probability** of data point i belonging to mixture component k .
- **M-step:** Use the **updated responsibilities** to **re-estimate** the parameters.

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- Intuitive idea: the log-likelihood is increased after each step.

EM algorithm for Estimating parameters of a GMM

- ① Initialize μ_k, Σ_k, π_k .
- ② **E-step:** Evaluate r_{ik} for every data point \mathbf{x}_i using the current parameters:

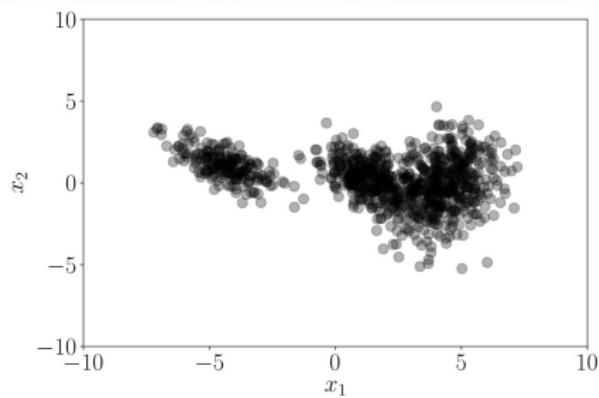
$$r_{ik} = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \mu_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_i | \mu_j, \Sigma_j)}$$

- ③ **M-step:** Re-estimate parameters μ_k, Σ_k, π_k using the current responsibilities r_{ik} from the E-step:

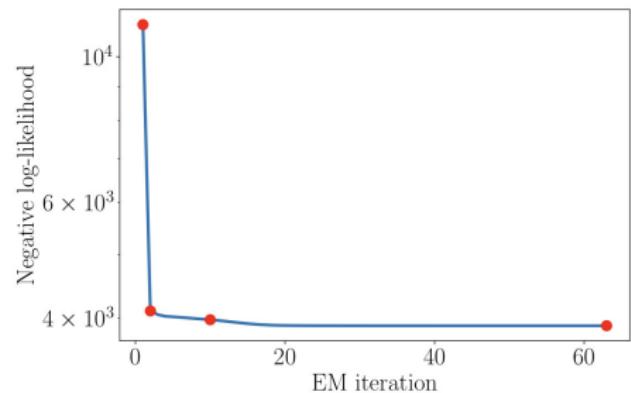
$$\mu_k = \frac{1}{N_k} \sum_{i=1}^N r_{ik} \mathbf{x}_i,$$

$$\Sigma_k = \frac{1}{N_k} \sum_{i=1}^N r_{ik} (\mathbf{x}_i - \mu_k)(\mathbf{x}_i - \mu_k)^\top,$$

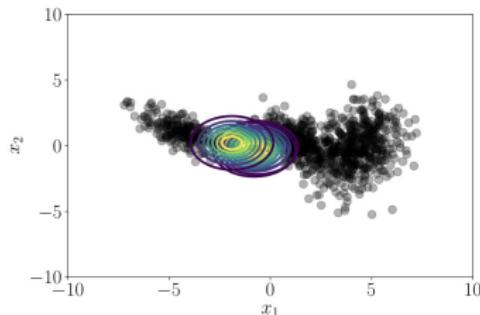
$$\pi_k = \frac{N_k}{N}.$$



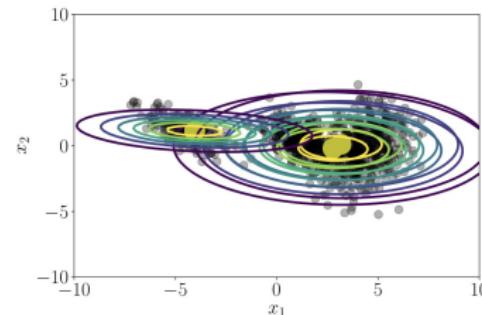
(a) Dataset.



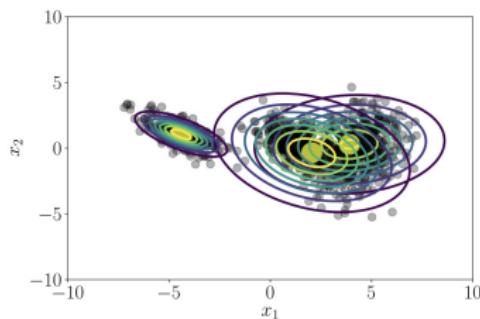
(b) Negative log-likelihood.



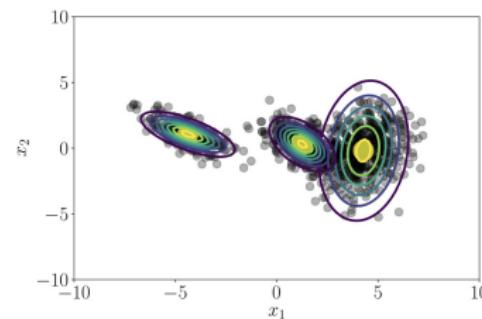
(c) EM initialization.



(d) EM after one iteration.



(e) EM after 10 iterations.



(f) EM after 62 iterations.

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Latent-Variable Perspective

- View the GMM from the perspective of a **discrete latent variable** model.
- The latent variable z can attain only a **finite** set of values.

A View of Generative Process

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- Define $\mathbf{z} := [z_1, z_2, \dots, z_K]^\top \in \mathbb{R}^K$ as a vector consisting of **exactly one 1 and $K - 1$ many 0s**.
 - One-hot encoding.
 - $\mathbf{z} = [z_1, z_2, z_3]^\top = [0, 1, 0]^\top \Rightarrow$ the 2nd mixture component is selected.

Prior on the latent variable

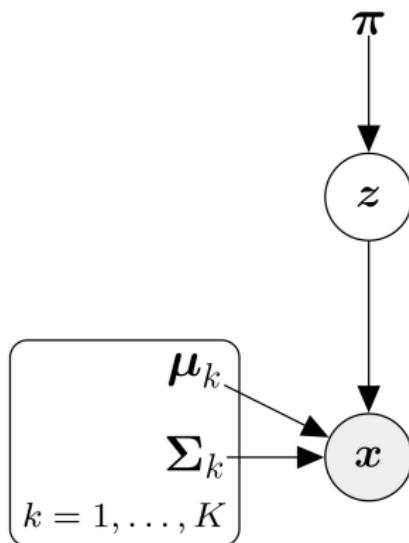
- When the variables z_k are unknown, we can place a prior distribution on \mathbf{z} in practice:

$$p(\mathbf{z}) = \boldsymbol{\pi} = [\pi_1, \pi_2, \dots, \pi_K]^\top, \sum_{k=1}^K \pi_k = 1,$$

where the k th entry $\pi_k = p(z_k = 1)$ describes the prob. that the k th mixture component generated data point \mathbf{x} .

Sampling from a GMM

Ancestral sampling.



A Simple Sampling Procedure

- ① Sample $z^{(i)} \sim p(\mathbf{z})$.
- ② Sample $\mathbf{x}^{(i)} \sim p(\mathbf{x} \mid z^{(i)} = 1)$.

Sampling from a GMM

The joint distribution

$$p(\mathbf{x}, z_k = 1) = p(\mathbf{x} | z_k = 1)p(z_k = 1) = \pi_k \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

for $k = 1, \dots, K$. So, we have

$$p(\mathbf{x}, \mathbf{z}) = \begin{bmatrix} p(\mathbf{x}, z_1 = 1) \\ p(\mathbf{x}, z_2 = 1) \\ \vdots \\ p(\mathbf{x}, z_K = 1) \end{bmatrix} = \begin{bmatrix} \pi_1 \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ \pi_2 \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\ \vdots \\ \pi_K \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_K), \end{bmatrix}$$

which fully specifies the probabilistic model.

Likelihood $p(\mathbf{x} | \boldsymbol{\theta})$ in a latent-variable model

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- Summing out (marginalizing out) all latent variables from $p(\mathbf{x}, \mathbf{z})$:

$$p(\mathbf{x} | \boldsymbol{\theta}) = \sum_{\mathbf{z}} p(\mathbf{x} | \boldsymbol{\theta}, \mathbf{z}) p(\mathbf{z} | \boldsymbol{\theta})$$

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$$\boldsymbol{\theta} := \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k : k = 1, 2, \dots, K\}.$$

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$$\boldsymbol{\theta} := \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k : k = 1, 2, \dots, K\}.$$

- There is only one single nonzero entry in each \mathbf{z} , so there are **only K possible configurations** of \mathbf{z} .

So, the desired marginal distribution is

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

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The latent variable model with latent indicators z_k is an equivalent way of thinking about a Gaussian mixture model.

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where the marginal $p(\mathbf{x}) = p(\mathbf{x} | \boldsymbol{\theta})$ is we have already derived.

- Hence,

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★ The responsibility of the k th mixture component for \mathbf{x} !

Extending to a Full Dataset (1/2)

- Consider a dataset of N data points $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$.
- Assume that every data point \mathbf{x}_i possesses its own latent variable

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$$p(\mathbf{x}_1, \dots, \mathbf{x}_N \mid \mathbf{z}_1, \dots, \mathbf{z}_N) = \prod_{i=1}^N p(\mathbf{x}_i \mid \mathbf{z}_i).$$

Extending to a Full Dataset (2/2)

Consider the posterior distribution $p(z_{ik} = 1 | \mathbf{x}_i)$ by applying Bayes' theorem:

$$\begin{aligned} p(z_{ik} = 1 | \mathbf{x}_i) &= \frac{p(\mathbf{x}_i | z_{ik} = 1)p(z_{ik} = 1)}{\sum_{j=1}^K p(\mathbf{x}_i | z_{ij} = 1)p(z_{ij} = 1)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \end{aligned}$$

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- Now, we see that the responsibilities have a mathematically justified interpretation as posterior probabilities.

GaussianMixture — scikit-learn [link]

The screenshot shows the scikit-learn API Reference for the GaussianMixture class. The left sidebar lists various modules like kernel_ridge, linear_model, manifold, metrics, and mixture. The mixture module is expanded, showing GaussianMixture and BayesianGaussianMixture. The main content area shows the GaussianMixture class definition, its purpose as a Gaussian mixture model, and a note that it was added in version 0.18. It also includes parameters for n_components and covariance_type.

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 - fit_predict
 - get_metadata_routing
 - get_params
 - predict
 - predict_proba
 - sample
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Discussions