

Mathematics for Machine Learning

— Gaussian Mixture Models

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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.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. 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 Introduction & Gaussian Mixture Model (GMM)
- 2 Parameter Learning via Maximum Likelihood
 - Updating the Means
 - Updating the Covariances
 - Updating the Mixture Weights

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1 Introduction & Gaussian Mixture Model (GMM)

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Introduction

Focus

- **Goal:** Density Estimation.
- Covering two important concepts:
 - Expectation maximization (EM).
 - Latent variable perspective.

Motivation

- A straightforward way to represent data: Let them present themselves directly.
- **Issue:** The data might be *dirty* or too huge to show all of them.

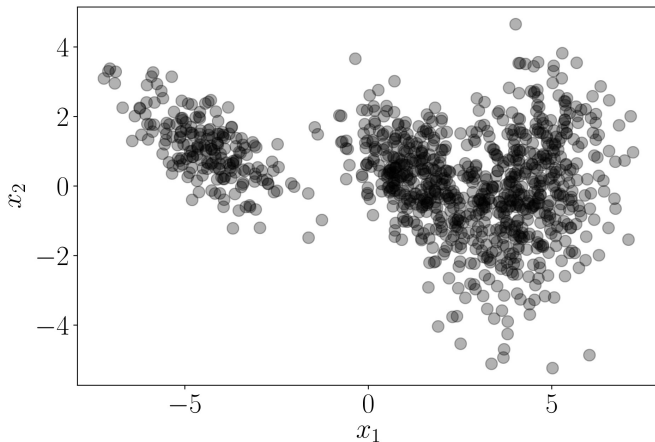
Motivation

- A straightforward way to represent data: Let them present themselves directly.
- **Issue:** The data might be *dirty* or too huge to show all of them.

We want to represent the data compactly using a density from a parametric family, such as Gaussian or Beta distribution.

- Mean & variance.

One Gaussian representation might not be meaningful.



A Solution

- Consider **mixture models**:
 - A convex combination of K simple base distributions.
 - A distribution $p(\mathbf{x})$:

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k p_k(\mathbf{x}),$$

$$0 \leq \pi_k \leq 1, \sum_{k=1}^K \pi_k = 1.$$

- π_k : *mixture weights*.
- More expressive than a base distribution.

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- π_k : *mixture weights*.
- More expressive than a base distribution.
- **Gaussian mixture models (GMMs)**: the base distributions are Gaussians.

Gaussian Mixture Model

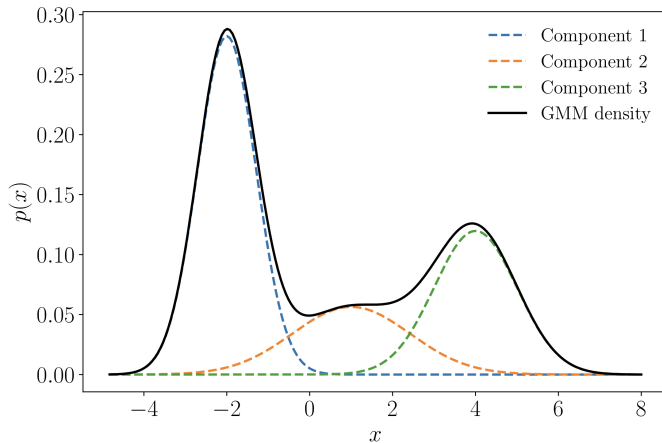
Gaussian Mixture Model

A Gaussian mixture model is a density model where we combine a finite number of K Gaussian distributions $\mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ such that

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$
$$0 \leq \pi_k \leq 1, \quad \sum_{k=1}^K \pi_k = 1,$$

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

GMMs



$$p(x | \theta) = 0.5\mathcal{N}(x | -2, 0.5) + 0.2\mathcal{N}(x | 1, 2) + 0.3\mathcal{N}(x | 4, 1).$$

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2 Parameter Learning via Maximum Likelihood

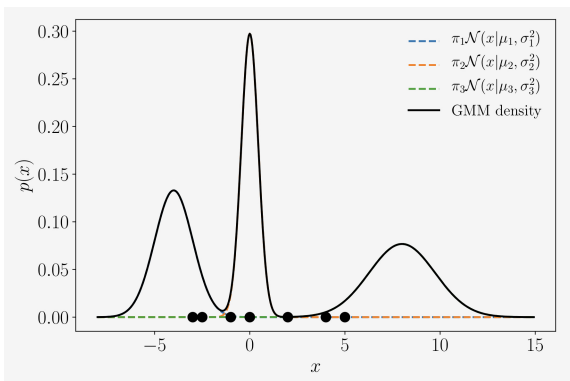
- Updating the Means
- Updating the Covariances
- Updating the Mixture Weights

The Setting

- A dataset $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$, where each \mathbf{x}_i is drawn i.i.d. from an unknown distribution $p(\mathbf{x})$.
- Parameters: $\theta := \{\mu_k, \Sigma_k, \pi_k \mid k = 1, \dots, K\}$.

Example of an Initial Setting

- $\mathcal{X} = \{-3, -2.5, -1, 0, 2, 4, 5\}$.
- $K = 3$.
- $p_1(x) = \mathcal{N}(x \mid -4, 1)$, $p_2(x) = \mathcal{N}(x \mid 0, 0.2)$, $p_3(x) = \mathcal{N}(x \mid 8, 3)$.
- $\pi_1 = \pi_2 = \pi_3 = 1/3$.



The Likelihood

By the i.i.d. assumption, we have the factorized likelihood

$$p(\mathcal{X} | \theta) = \prod_{i=1}^N p(\mathbf{x}_i | \theta), \quad p(\mathbf{x}_i | \theta) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

Then the log-likelihood is

$$\mathcal{L} := \log p(\mathcal{X} | \theta) = \sum_{i=1}^N \log p(\mathbf{x}_i | \theta) = \sum_{i=1}^N \log \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

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- **Goal:** Find parameters θ_{ML}^* .

MLE

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- We cannot obtain a closed-form solution here (except for $K = 1$, i.e., single Gaussian).
- We exploit an iterative scheme to find θ_{ML}^* : the EM algorithm.
- **The key idea:** Update one model parameter at a time while keeping the others fixed.

Necessary conditions for a local optimum of \mathcal{L} :

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top &\iff \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top \\ \frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0}^\top &\iff \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0}^\top \\ \frac{\partial \mathcal{L}}{\partial \pi_k} = 0 &\iff \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \pi_k} = 0.\end{aligned}$$

Applying the chain rule:

$$\frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{1}{p(\mathbf{x}_i | \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$$

and

$$\frac{1}{p(\mathbf{x}_i | \boldsymbol{\theta})} = \frac{1}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.$$

Responsibilities: Facilitating our discussions

Responsibility of the k th mixture component for n th data point

$$r_{ik} := \frac{\pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.$$

- Note that

$$p(\mathbf{x}_i \mid \pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

which is proportional to the likelihood.

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- High responsibility \implies The data point is plausible sample from that mixture component.

Remark

$\mathbf{r}_i := [r_{i1}, \dots, r_{iK}]^\top \in \mathbb{R}^K$ is a normalized probability vector.

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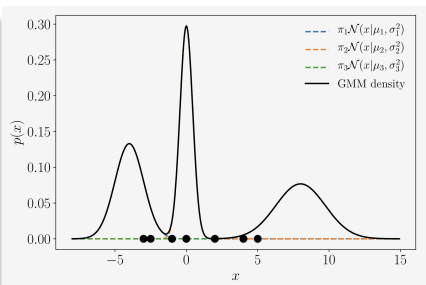
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- A *soft assignment* of \mathbf{x}_i to the K mixture component.
 - Similar idea: softmax functions.

Example (responsibilities of the previous example)

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.057 & 0.943 & 0.0 \\ 0.001 & 0.999 & 0.0 \\ 0.0 & 0.066 & 0.934 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 1.0 \end{bmatrix} \in \mathbb{R}^{N \times K}.$$

- Try to compute it by yourselves.



Update of the GMM Means

Theorem [Update of the Means]

The update of the mean parameters μ_k , $k = 1, \dots, K$, of the GMM is given by

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

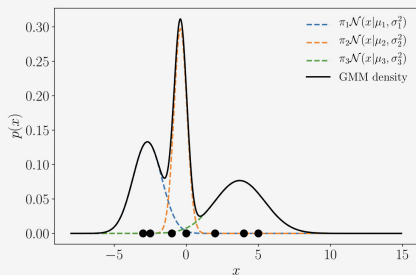
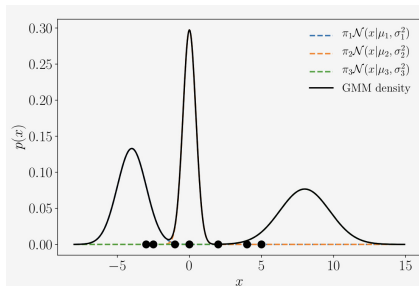
$$\begin{aligned}
 \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} &= \sum_{j=1}^K \pi_j \frac{\partial \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\partial \boldsymbol{\mu}_k} = \pi_k \frac{\partial \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k,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

$$\begin{aligned}
 \frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} &= \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^N \frac{1}{p(\mathbf{x}_i | \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} \\
 &= \sum_{i=1}^N (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \\
 &= \sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}.
 \end{aligned}$$

$$\text{Solving } \frac{\partial \mathcal{L}(\boldsymbol{\mu}_k^{\text{new}})}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k^{\text{new}})^\top \boldsymbol{\Sigma}_k^{-1} = \mathbf{0}^\top:$$

$$\begin{aligned} \sum_{i=1}^N r_{ik} \mathbf{x}_i &= \sum_{i=1}^N r_{ik} \boldsymbol{\mu}_k^{\text{new}} \\ \iff \boldsymbol{\mu}_k^{\text{new}} &= \frac{\sum_{i=1}^N r_{ik} \mathbf{x}_i}{\sum_{i=1}^N r_{ik}} = \frac{1}{N_k} \sum_{i=1}^N r_{ik} \mathbf{x}_i, \end{aligned}$$

where $N_k := \sum_{i=1}^N r_{ik}$.



- $\mu_1 : -4 \rightarrow -2.7$.
- $\mu_2 : 0 \rightarrow -0.4$.
- $\mu_3 : 8 \rightarrow 3.7$.

Remark

- r_{ik} is a function of π_j, μ_j, Σ_j for all $j = 1, \dots, K$.
- Hence the updates depend on all parameters of the GMM.

Update of the GMM Covariances

Theorem [Update of the Covariances]

The update of the covariance parameters Σ_k , $k = 1, \dots, K$, of the GMM is given by

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

where

$$r_{ik} := \frac{\pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_j, \Sigma_j)}.$$

and $N_k := \sum_{i=1}^N r_{ik}$.

$$\frac{\partial \mathcal{L}}{\partial \Sigma_k} = \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \Sigma_k} = \sum_{i=1}^N \frac{1}{p(\mathbf{x}_i | \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \Sigma_k}$$

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$$\begin{aligned} \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \Sigma_k} &= \frac{\partial}{\partial \Sigma_k} \left(\pi_k (2\pi)^{-\frac{D}{2}} \det(\Sigma_k)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) \right) \\ &= \pi_k (2\pi)^{-\frac{D}{2}} \left[\frac{\partial}{\partial \Sigma_k} \det(\Sigma_k)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) \right. \\ &\quad \left. + \det(\Sigma_k)^{-\frac{1}{2}} \frac{\partial}{\partial \Sigma_k} \exp \left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) \right] \end{aligned}$$

Note that

$$\begin{aligned} \frac{\partial}{\partial \Sigma_k} \det(\Sigma_k)^{-\frac{1}{2}} &= -\frac{1}{2} \det(\Sigma_k)^{-\frac{1}{2}} \Sigma_k^{-1}, \\ \frac{\partial}{\partial \Sigma_k} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) &= -\Sigma_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1} \end{aligned}$$

$$\frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \cdot \left[-\frac{1}{2} (\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \right]$$

Thus,

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} &= \sum_{i=1}^N \frac{\partial \log p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \sum_{i=1}^N \frac{1}{p(\mathbf{x}_i | \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} \\ &= \sum_{i=1}^N \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \\ &\quad \cdot \left[-\frac{1}{2} (\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \right] \\ &= -\frac{1}{2} \sum_{i=1}^N r_{ik} (\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \\ &= -\frac{1}{2} \left(\sum_{i=1}^N r_{ik} \right) \boldsymbol{\Sigma}_k^{-1} + \frac{1}{2} \boldsymbol{\Sigma}_k^{-1} \left(\sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \right) \boldsymbol{\Sigma}_k^{-1}. \end{aligned}$$

$$\frac{\partial p(\mathbf{x}_i | \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \cdot \left[-\frac{1}{2} (\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \right]$$

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Setting $\frac{\partial \mathcal{L}}{\partial \Sigma_k} = \mathbf{0}^\top$, we have

$$N_k \Sigma_k^{-1} = \Sigma_k^{-1} \left(\sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \right) \Sigma_k^{-1}$$

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Then,

$$N_k \mathbf{I} = \Sigma_k^{-1} \left(\sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \right)$$

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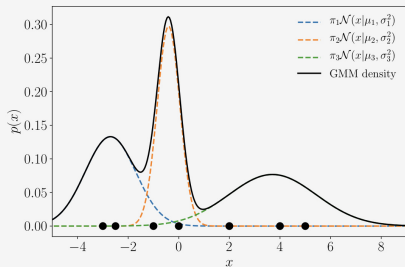
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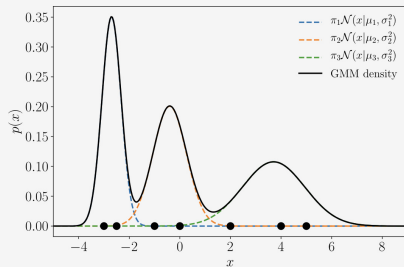
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Hence,

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^N r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top.$$



(a) GMM density and individual components prior to updating the variances.



(b) GMM density and individual components after updating the variances.

- $\sigma_1^2 : 1 \rightarrow 0.14$.
- $\sigma_2^2 : 0.2 \rightarrow 0.44$.
- $\sigma_3^2 : 3 \rightarrow 1.53$.

Update of the GMM Mixture Weights

Theorem [Update of the Mixture Weights]

The update of the mixture weights of the GMM is given by

$$\pi_k^{\text{new}} = \frac{N_k}{N}, \quad k = 1, \dots, K.$$

- N : the number of data points.
- $N_k := \sum_{i=1}^N r_{ik}$.

- We account for the constraint $\sum_k \pi_k = 1$.
 - Using Lagrange multipliers.

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 - Using Lagrange multipliers.
- The Lagrangian:

$$\begin{aligned}\mathfrak{L} &= \mathcal{L} + \lambda \left(\sum_{k=1}^K \pi_k - 1 \right) \\ &= \sum_{i=1}^N \log \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) + \lambda \left(\sum_{k=1}^K \pi_k - 1 \right).\end{aligned}$$

Obtain the partial derivative of \mathcal{L} w.r.t. π_k :

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \pi_k} &= \sum_{i=1}^N \frac{\mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} + \lambda \\ &= \frac{1}{\pi_k} \sum_{i=1}^N \frac{\pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} + \lambda \\ &= \frac{N_k}{\pi_k} + \lambda,\end{aligned}$$

and the partial derivative w.r.t. λ is

$$\frac{\partial \mathcal{L}}{\partial \lambda} = \sum_{k=1}^K \pi_k - 1.$$

Now we have

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \frac{N_k}{\pi_k} + \lambda$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = \sum_{k=1}^K \pi_k - 1$$

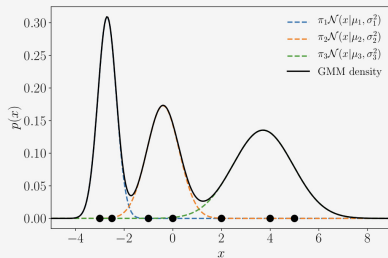
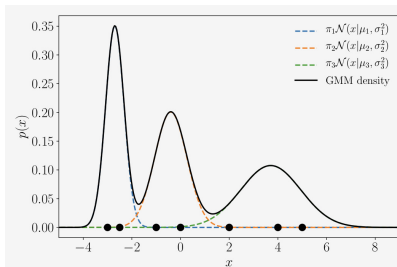
Now we have

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \frac{N_k}{\pi_k} + \lambda$$
$$\frac{\partial \mathcal{L}}{\partial \lambda} = \sum_{k=1}^K \pi_k - 1$$

Setting both to $\mathbf{0}^\top$ we have

$$\pi_k = -\frac{N_k}{\lambda}$$
$$1 = \sum_{k=1}^K \pi_k = -\sum_{k=1}^K \frac{N_k}{\lambda} = -\frac{N}{\lambda}$$

So $\lambda = -N \implies \pi_k^{new} = \frac{N_k}{N}$.



- $\pi_1 : \frac{1}{3} \rightarrow 0.29$.
- $\pi_2 : \frac{1}{3} \rightarrow 0.29$.
- $\pi_3 : \frac{1}{3} \rightarrow 0.42$.

Discussions