Mathematics for Machine Learning

— Density Estimation with 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

Outline

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.

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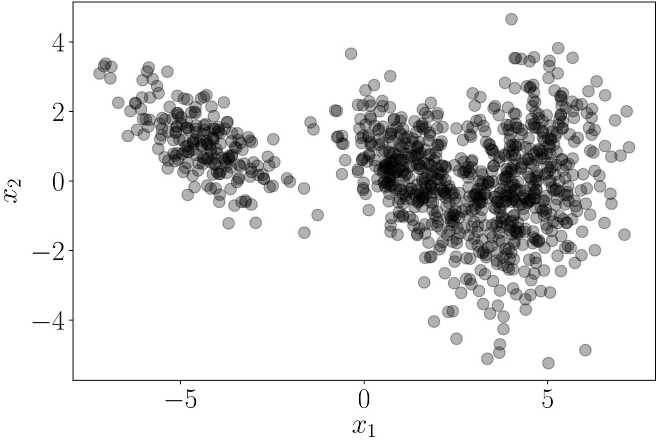
- **Issue:** The data might be *dirty* or too huge to show all of them.

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

A Gaussian approximation of the density might be poor.



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 modesl (GMMs): the base distributions are Gaussians.

Gaussian Mixture Model

Gaussian Mixture Model

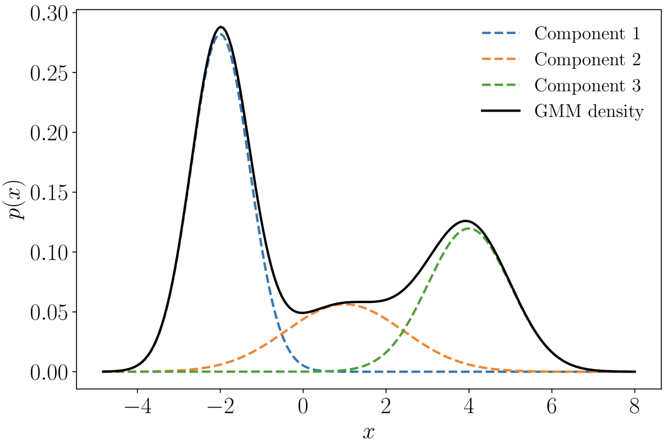
A Gaussian mixture model is a density model where we combine a finite number of K Gaussian distributions $\mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ such that

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

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

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

GMMs



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

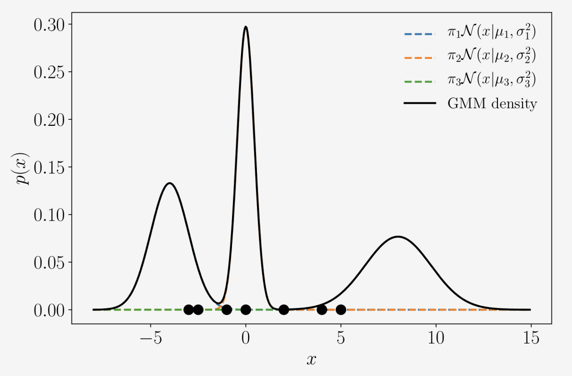
Outline

The Setting

- A dataset $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$, where each x_i is drawn i.i.d. from an unknown distribution $p(\mathbf{x})$.
- Unknown distribution $p(\mathbf{x})$
- Parameters: $\boldsymbol{\theta} := \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k \mid k = 1, \ldots, K\}$.

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

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

Then the log-likelihood is

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

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- **Goal:** Find parameters $\boldsymbol{\theta}^*_{ML}$.

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 $\boldsymbol{\theta}^*_{ML}$: 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 $\mathcal{L}$:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top \iff \sum_{i=1}^{N} \frac{\partial \log p(\mathbf{x}_i \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0}^\top \iff \sum_{i=1}^{N} \frac{\partial \log p(\mathbf{x}_i \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0}^\top$$

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \mathbf{0}^\top \iff \sum_{i=1}^{N} \frac{\partial \log p(\mathbf{x}_i \mid \boldsymbol{\theta})}{\partial \pi_k} = 0.$$

Applying the chain rule:

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

and

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

Responsibilities: Facilitating our discussions

Responsibility of the kth mixture conponent for nth 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

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

which is proportional to the likelihood.

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which is proportional to the likelihood.
- High responsibility $\Longrightarrow$ The data point is plausible sample from that mixture component.

Remark

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

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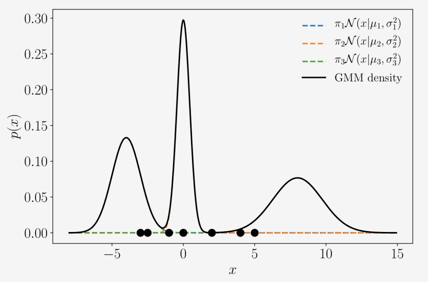
- A *soft assignment* of $\mathbf{x}_n$ to the K mixture component.
    - Similar idea: softmax functions.

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 $\boldsymbol{\mu}_k$, $k = 1, \ldots, K$, of the GMM is given by

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

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

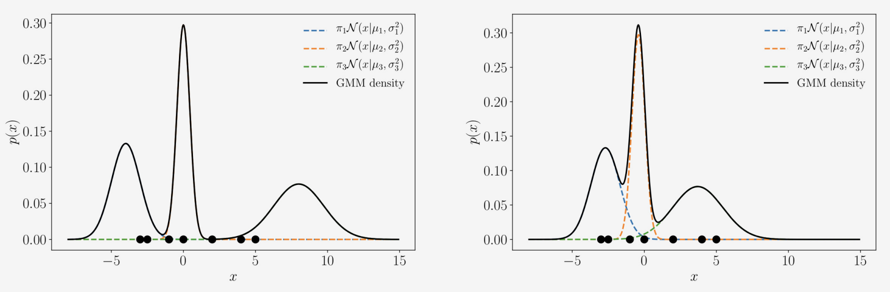
$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^{N} \frac{\partial \log p(\mathbf{x}_i \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^{N} \frac{1}{p(\mathbf{x}_i \mid \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i \mid \boldsymbol{\theta})}{\partial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

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

$$\sum_{i=1}^{N} r_{ik}\mathbf{x}_i = \sum_{i=1}^{N} r_{ik}\boldsymbol{\mu}^{new}$$

$$\iff \quad \boldsymbol{\mu}_k^{new} = \frac{\sum_{i=1}^{N} r_{ik}\mathbf{x}_i}{\sum_{i=1}^{N} r_{ik}} = \frac{1}{N_k}\sum_{i=1}^{N} r_{ik}\mathbf{x}_i,$$

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



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

Remark

- r_{ik} is a function of $\pi_j, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j$ for all $j = 1, \ldots, K$.
- 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 $\boldsymbol{\Sigma}_k$, $k = 1, \ldots, K$, of the GMM is given by

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

where

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

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

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

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

Note that

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

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

Thus,

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

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

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&\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} \boldsymbol{\Sigma}_k^{-1} N_k + \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}$$

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

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

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Then,

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

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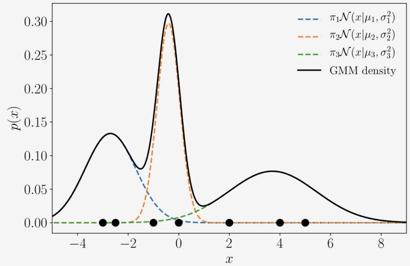
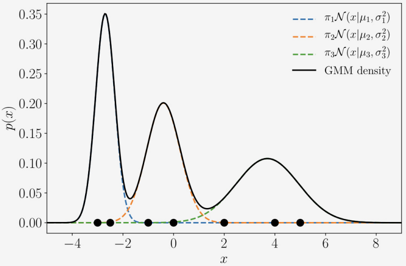
Hence,

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



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



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

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

Update of the GMM Mixture Weights

Theorem [Update of the Mixture Weights]

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

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

- 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 $\mathfrak{L}$ w.r.t. π_k:

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

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

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

Now we have

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

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

Now we have

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

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

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

Now we have

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

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

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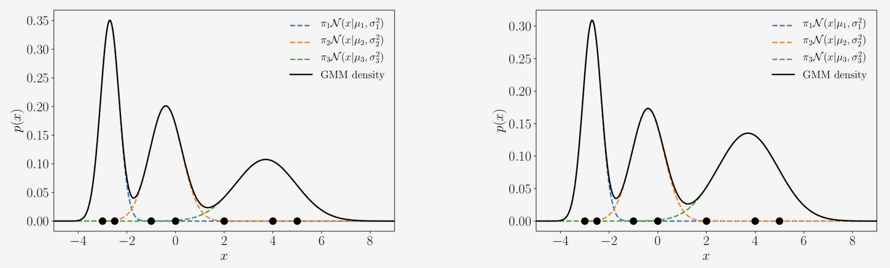

- $\pi_1 : \frac{1}{3} \to 0.29.$
- $\pi_2 : \frac{1}{3} \to 0.29.$
- $\pi_3 : \frac{1}{3} \to 0.42.$

Outline

Motivation

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  - $\because$ 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

Dempster et al. (1977)

Choose initial parameter values (i.e., $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$) and alternate between the following two steps until convergence:

- E-step: Evaluate the responsibilities r_{ik}
  - It can be viewed as the posterior prob. of data point i belonging to mixture component k.
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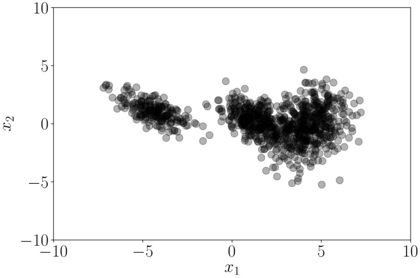
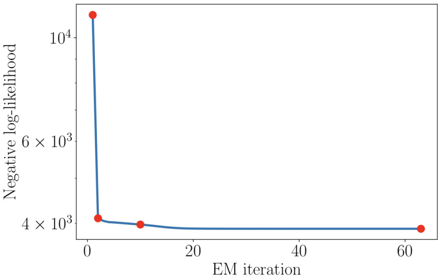
- Intuitive idea: the log-likelihood is increased after each step.

EM algorithm for Estimating parameters of a GMM

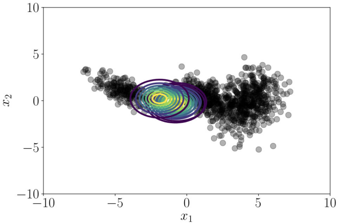
1. Initialize $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$.
2. **E-step**: Evaluate r_{ik} for every data point $\mathbf{x}_i$ using the current parameters:
$$r_{ik} = \frac{\pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$
3. **M-step**: Re-estimate parameters $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$ using the current responsibilities r_{ik} from the E-step:
$$\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k} \sum_{i=1}^{N} r_{ik} \mathbf{x}_i, \\
\boldsymbol{\Sigma}_k &= \frac{1}{N_k} \sum_{i=1}^{N} r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top, \\
\pi_k &= \frac{N_k}{N}.
\end{aligned}$$



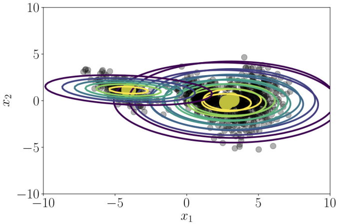
(a) Dataset.



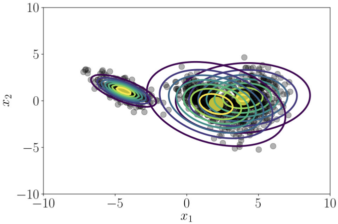
(b) Negative log-likelihood.



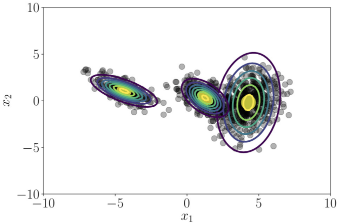
(c) EM initialization.



(d) EM after one iteration.



(e) EM after 10 iterations.



(f) EM after 62 iterations.

Outline

Latent-Variable Perspective

- View the GMM from the perspective of a discrete latent variable model.
- The latent variable $\mathbf{z}$ can attain only a finite set of values.

A View of Generative Process

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- Define $\mathbf{z} := [z_1, \ldots, z_K]^\top \in \mathbb{R}^K$ 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.

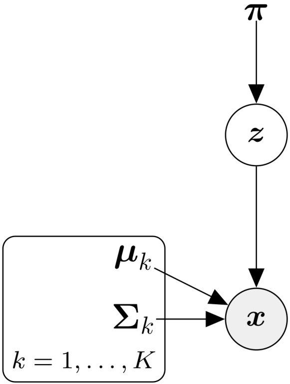
Prior on the latent variable

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

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

where the kth entry $\pi_k = p(z_k = 1)$ describes the prob. that the kth 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

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

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

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

which fully specifies the probabilistic model.

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

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

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

- 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

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which is exactly the GMM likelihood we have derived before!

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  - ⋆ The responsibility of the kth mixture component for $\mathbf{x}$!

Extending to a Full Dataset (1/2)

- Consider a dataset of N data points $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$.
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Consider the posterior distribution $p(z_{ik} = 1 \mid \mathbf{x}_i)$ by applying Bayes' theorem:

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&= \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)}
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- Now, we see that the responsibilities have a mathematically justified interpretation as posterior probabilities.

Discussions