Mathematics for Machine Learning
— Expectation Maximization

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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

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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

- 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., $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$) and **alternate** between the following two steps until convergence:

- E-step: Evaluate the responsibilities r_{ik}
  - It can be viewed as the posterior 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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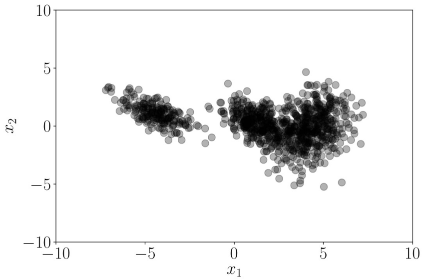
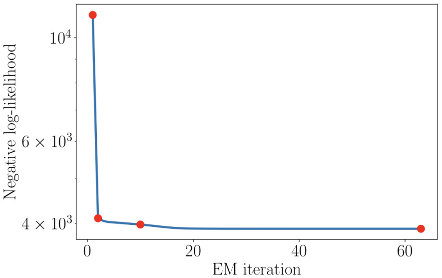
- Intuitive idea: the log-likelihood is increased after each step.

EM algorithm for Estimating parameters of a GMM

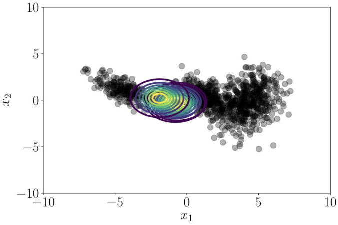
1. Initialize $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$.
2. **E-step**: Evaluate r_{ik} for every data point $\mathbf{x}_i$ using the current parameters:
$$r_{ik} = \frac{\pi_k \mathcal{N}(\mathbf{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_i \mid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



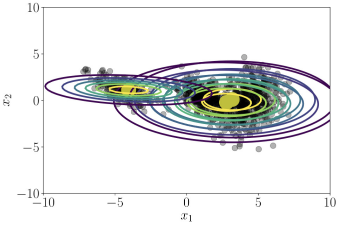
(a) Dataset.



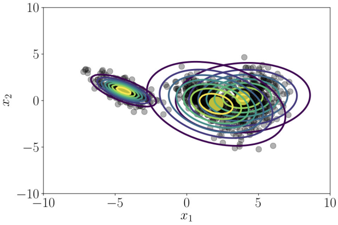
(b) Negative log-likelihood.



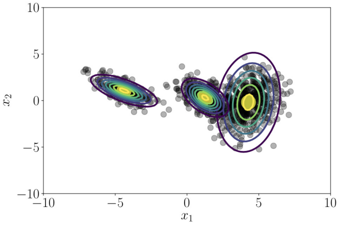
(c) EM initialization.



(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 $\mathbf{z} := [z_1, z_2, \ldots, z_K]^\top \in \mathbb{R}^K$ 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.

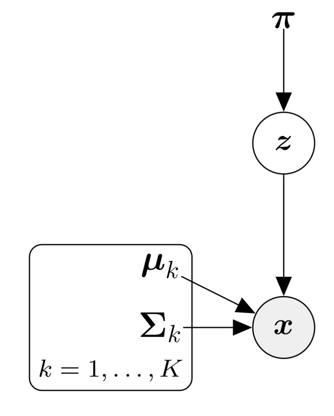
Prior on the latent variable

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

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

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

Previously, we omitted the parameters $\boldsymbol{\theta}$ of the probabilistic model.

- How to obtain the likelihood $p(\mathbf{x} \mid \boldsymbol{\theta})$ in a latent-variable model?

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

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

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

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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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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 $p(\mathbf{x}) = p(\mathbf{x} \mid \boldsymbol{\theta})$ is we have already derived.

- Hence,

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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 $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$.
- Assume that every data point $\mathbf{x}_i$ possesses its own latent variable

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Extending to a Full Dataset (2/2)

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

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

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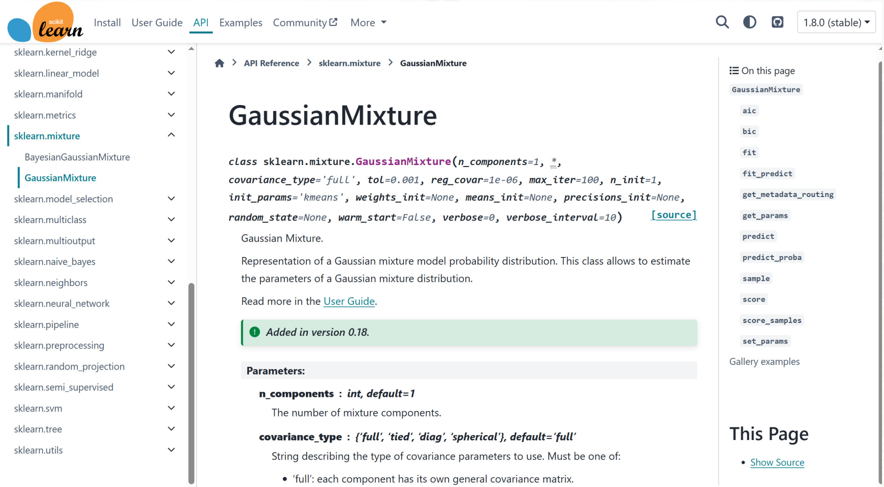
$$

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

GaussianMixture — scikit-learn [link]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sklearn.kernel_ridge
sklearn.linear_model
sklearn.manifold
sklearn.metrics
sklearn.mixture
BayesianGaussianMixture
GaussianMixture
sklearn.model_selection
sklearn.multiclass
sklearn.multioutput
sklearn.naive_bayes
sklearn.neighbors
sklearn.neural_network
sklearn.pipeline
sklearn.preprocessing
sklearn.random_projection
sklearn.semi_supervised
sklearn.svm
sklearn.tree
sklearn.utils

API Reference > sklearn.mixture > GaussianMixture

GaussianMixture

class `sklearn.mixture.GaussianMixture(n_components=1, *, covariance_type='full', tol=0.001, reg_covar=1e-06, max_iter=100, n_init=1, init_params='kmeans', weights_init=None, means_init=None, precisions_init=None, random_state=None, warm_start=False, verbose=0, verbose_interval=10)` [source]

Gaussian Mixture.

Representation of a Gaussian mixture model probability distribution. This class allows to estimate the parameters of a Gaussian mixture distribution.

Read more in the User Guide.

Added in version 0.18.

Parameters:

n_components : *int, default=1*

The number of mixture components.

covariance_type : *{'full', 'tied', 'diag', 'spherical'}, default='full'*

String describing the type of covariance parameters to use. Must be one of:

- 'full': each component has its own general covariance matrix.

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get_params
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