CS 6316 Machine Learning

Generative Models

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Basic Definition

Data generation process

An idealized process to illustrate the relations among domain set $\mathcal{X}$, label set $\mathcal{Y}$, and the training set S

1. the probability distribution $\mathcal{D}$ over the domain set $\mathcal{X}$
2. sample an instance $\boldsymbol{x} \in \mathcal{X}$ according to $\mathcal{D}$
3. annotate it using the labeling function f as $y = f(\boldsymbol{x})$

[From Lecture 02]

Example

Here is an data generation model

$$p(\boldsymbol{x}) = \underbrace{0.6 \cdot \mathcal{N}(x; \boldsymbol{\mu}_+, \boldsymbol{\Sigma}_+)}_{y=+1} + \underbrace{0.4 \cdot \mathcal{N}(x; \boldsymbol{\mu}_-, \boldsymbol{\Sigma}_-)}_{y=-1} \tag{1}$$

with

- $\boldsymbol{\mu}_+ = [2, 0]^\top$
- $\boldsymbol{\Sigma}_+ = \begin{bmatrix} 1.0 & 0.8 \\ 0.8 & 2.0 \end{bmatrix}$
- $\boldsymbol{\mu}_- = [-2, 0]^\top$
- $\boldsymbol{\Sigma}_- = \begin{bmatrix} 2.0 & 0.6 \\ 0.6 & 1.0 \end{bmatrix}$

Example (II)

The data generation model can also be represented with the following components

$$
\begin{aligned}
p(y = +1) &= 0.6 && (2)\\
p(y = -1) &= 1 - p(y = +1) = 0.4 && (3)\\
p(\boldsymbol{x} \mid y = +1) &= \mathcal{N}(x; \boldsymbol{\mu}_{+}, \boldsymbol{\Sigma}_{+}) && (4)\\
p(\boldsymbol{x} \mid y = -1) &= \mathcal{N}(x; \boldsymbol{\mu}_{-}, \boldsymbol{\Sigma}_{-}) && (5)
\end{aligned}
$$

Data Generation

The specific data generation process:
for each data point

1. Randomly select a value of $y \in \{+1, -1\}$ based on

$$p(y = +1) = 0.6 \quad p(y = -1) = 0.4 \tag{6}$$

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2. Sample $\boldsymbol{x}$ from the corresponding component based on the value of y

$$p(\boldsymbol{x} \mid y) = \begin{cases} \mathcal{N}(x; \boldsymbol{\mu}_{+}, \boldsymbol{\Sigma}_{+}) & y = +1 \\ \mathcal{N}(x; \boldsymbol{\mu}_{-}, \boldsymbol{\Sigma}_{-}) & y = -1 \end{cases} \tag{7}$$

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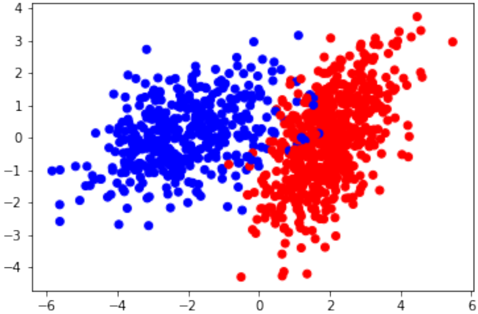
3. Add $(\boldsymbol{x}, y)$ to S, go to step 1

Illustration

With $N = 1000$ samples, here is the plot



- 588 positive samples and 412 negative samples

Discriminative Models for Classification

- Discriminative models directly give predictions on the target variable (e.g., y)
- Example: logistic regression

$$p(y \mid \boldsymbol{x}) = \sigma(y\langle \boldsymbol{w}, \boldsymbol{x}\rangle) = \frac{1}{1 + e^{-y\langle \boldsymbol{w}, \boldsymbol{x}\rangle}} \tag{8}$$

where $\boldsymbol{w}$ is the model parameter

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- Other examples
  - AdaBoost (lecture 05)
  - SVMs (lecture 07)
  - Feed-forward neural network (lecture 08)

Generative Models for Classification

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- For the binary classification problem, recall the basic components of the data generation process
  - $p(y)$ where $y \in \{-1, +1\}$
  - $p(\boldsymbol{x} \mid y = +1)$ where $\boldsymbol{x} \in \mathbb{R}^d$
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  - $p(\boldsymbol{x} \mid y = -1)$ where $\boldsymbol{x} \in \mathbb{R}^d$
- Challenge in machine learning: we do not know any of them, instead we have the samples S from this distribution
  - This has always been our assumption in machine learning — we have no idea about the true data distribution

Generative Models for Classification (II)

We use a set of distribution $q(\cdot)$ to approximate the true distribution $p(\cdot)$

Data Generation Model	Generative Model
$p(y)$	$q(y)$
$p(\boldsymbol{x} \mid y = +1)$	$q(\boldsymbol{x} \mid y = +1)$
$p(\boldsymbol{x} \mid y = -1)$	$q(\boldsymbol{x} \mid y = -1)$

Learning with Generative Models

1. Define distributions for all components
2. Estimate the parameters for each component distribution

Defining Distributions

A typical way of defining distributions for generative models is based on *our understanding about the problem*

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- Output domain $y \in \{+1, -1\}$: **Bernoulli** distribution

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  where $\boldsymbol{\mu}_+$ and $\boldsymbol{\Sigma}_+$ are the parameters
- Similarly, for $p(\boldsymbol{x} \mid y = -1)$

$$p(\boldsymbol{x} \mid y = -1) = \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_-, \boldsymbol{\Sigma}_-) \tag{11}$$

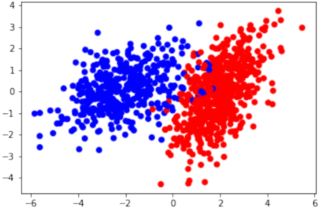
  where $\boldsymbol{\mu}_-$ and $\boldsymbol{\Sigma}_-$ are the parameters

Parameter Estimation

- The collection of the parameters

$$\theta = \{\alpha, \boldsymbol{\mu}_{+}, \boldsymbol{\Sigma}_{+}, \boldsymbol{\mu}_{\text{-}}, \boldsymbol{\Sigma}_{\text{-}}\} \tag{12}$$

- Training data $S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$



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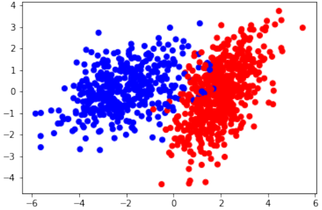

- Learning algorithm: Maximum Likelihood Estimation (MLE)

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MLE defined on the whole distribution $q(\boldsymbol{x}, y)$

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Based on the chain rule of probability

$$q(\boldsymbol{x}, y; \boldsymbol{\theta}) = q(y; \alpha) q(\boldsymbol{x} \mid y; \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y), \tag{14}$$

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Therefore

$$\hat{\boldsymbol{\theta}} \leftarrow \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \left\{ \sum_{i=1}^{m} \log \log q(y_i; \alpha) + \sum_{i=1}^{m} \log q(\boldsymbol{x}_i \mid y_i; \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y) \right\}$$

the last item has two components, depending on the value of y

MLE: Bernoulli Distribution

Recall the definition of Bernoulli distribution, we have

$$\sum_{i=1}^{m} \log q(y_i;\alpha) = \sum_{i=1}^{m} \{\delta(y_i = +1)\log\alpha + \delta(y_i = -1)\log(1-\alpha)\} \tag{15}$$

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Then, the value of α can be estimated from

$$\frac{d\sum_{i=1}^{m}\log q(y_i;\alpha)}{d\alpha} = \frac{\sum_{i=1}^{m}\delta(y_i = +1)}{\alpha} - \frac{\sum_{i=1}^{m}\delta(y_i = -1)}{1-\alpha} = 0 \tag{16}$$

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therefore,

$$\alpha = \frac{\sum_{i=1}^{m} \delta(y_i = +1)}{m} \tag{17}$$

MLE: Gaussian Distribution

The definition of multi-variate Gaussian distribution

$$q(\boldsymbol{x} \mid y; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\top}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right) \quad (18)$$

- For $y = +1$, MLE on $\boldsymbol{\mu}_+$ and $\boldsymbol{\Sigma}_+$ will only consider the samples $\boldsymbol{x}$ with $y = +1$ (assume it's S_+)

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$$\boldsymbol{\mu} = \frac{1}{|S_+|} \sum_{\boldsymbol{x}_i \in S_+} \boldsymbol{x}_i \quad (19)$$

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$$q(\boldsymbol{x} \mid y; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right) \quad (18)$$

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- MLE on $\boldsymbol{\Sigma}_+$

$$\boldsymbol{\Sigma}_+ = \frac{1}{|S_+|} \sum_{\boldsymbol{x}_i \in S_+} (\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^{\mathsf{T}} \quad (20)$$

- *Exercise*: prove equations 19 and 20 with $d = 1$

Example: Parameter Estimation

Given $N = 1000$ samples, here are the parameters

Parameter	$p(\cdot)$	$q(\cdot)$
$\boldsymbol{\mu}_+$	$[2, 0]^\mathsf{T}$	$[1.95, -0.11]^\mathsf{T}$
$\boldsymbol{\Sigma}_+$	$\begin{bmatrix} 1.0 & 0.8 \\ 0.8 & 2.0 \end{bmatrix}$	$\begin{bmatrix} 0.88 & 0.74 \\ 0.74 & 1.97 \end{bmatrix}$
$\boldsymbol{\mu}_-$	$[-2, 0]^\mathsf{T}$	$[-2.08, 0.08]^\mathsf{T}$
$\boldsymbol{\Sigma}_-$	$\begin{bmatrix} 2.0 & 0.6 \\ 0.6 & 1.0 \end{bmatrix}$	$\begin{bmatrix} 1.88 & 0.55 \\ 0.55 & 1.07 \end{bmatrix}$

Prediction

- For a new data point $\boldsymbol{x}'$, the prediction is given as

$$q(y' \mid \boldsymbol{x}') = \frac{q(y')q(\boldsymbol{x} \mid y')}{q(\boldsymbol{x}')} \propto q(y')q(\boldsymbol{x}' \mid y') \qquad (21)$$

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- Prediction rule

$$y' = \begin{cases} +1 & q(y' = +1 \mid \boldsymbol{x}') > q(y' = -1 \mid \boldsymbol{x}') \\ -1 & q(y' = +1 \mid \boldsymbol{x}') < q(y' = +1 \mid \boldsymbol{x}') \end{cases} \tag{22}$$

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- Although equation 22 looks like the one used in the Bayes optimal predictor, the prediction power is limited by

$$q(y' \mid \boldsymbol{x}') \approx p(y \mid \boldsymbol{x}) \tag{23}$$

  Again, we don't know $p(\cdot)$

Naive Bayes Classifiers

Number of Parameters

Assume $\boldsymbol{x} = (x_{\cdot,1}, \ldots, x_{\cdot,d}) \in \mathbb{R}^d$, then the number of parameters in $q(\boldsymbol{x}, y)$

- $q(y)$: 1 (α)
- $q(\boldsymbol{x} \mid y = +1)$:
  - $\boldsymbol{\mu}_+ \in \mathbb{R}^d$: d parameters
  - $\boldsymbol{\Sigma}_+ \in \mathbb{R}^{d \times d}$: d^2 parameters
- $q(\boldsymbol{x} \mid y = -1)$: $d^2 + d$ parameters

In total, we have $2d^2 + 2d + 1$ parameters

Challenge of Parameter Estimation

- When $d = 100$, we have $2d^2 + 2d + 1 = 20201$ parameters
- A close look about the covariance matrix $\mathbf{\Sigma}$ in a multivariate Gaussian distribution

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_{1,1}^2 & \cdots & \sigma_{1,d}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{d,1}^2 & \cdots & \sigma_{d,d}^2 \end{bmatrix} \tag{24}$$

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- To reduce the number of parameters, we assume

$$\sigma_{i,j} = 0 \quad \text{if } i \neq j \tag{25}$$

Diagonal Covariance Matrix

With the diagonal covariance matrix

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_{1,1}^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_{d,d}^2 \end{bmatrix} \tag{26}$$

Now, the multivariate Gaussian distribution can be rewritten with

$$|\mathbf{\Sigma}| = \prod_{j=1}^{d} \sigma_{j,j}^2 \tag{27}$$

$$(\boldsymbol{x} - \boldsymbol{\mu})^\mathsf{T} \mathbf{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) = \sum_{j=1}^{d} \frac{(x_{\cdot,j} - \mu_j)^2}{\sigma_{j,j}^2} \tag{28}$$

Diagonal Covariance Matrix (II)

In other words

$$q(\boldsymbol{x} \mid y, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{j=1}^{d} q(x_{\cdot,j} \mid y; \mu_j, \sigma^2_{j,j}) \tag{29}$$

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- Parameter estimation can be done per dimension

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Latent Variable Models

Data Generation Model, Revisited

Consider the following model again without any label information

$$p(\boldsymbol{x}) = \underbrace{\alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)}_{c=1} + \underbrace{(1-\alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)}_{c=2} \qquad (30)$$

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- No labeling information
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- Instead of having two classes, now it has two components $c \in \{1, 2\}$
- It is a specific case of *Gaussian mixture models*
  - A mixture model with two Gaussian components

Data Generation

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1. Randomly select a component c based on

$$p(c = 1) = \alpha \quad p(c = 2) = 1 - \alpha \tag{31}$$

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2. Sample $\boldsymbol{x}$ from the corresponding component c

$$p(\boldsymbol{x} \mid y) = \begin{cases} \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) & c = 1 \\ \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) & c = 2 \end{cases} \tag{32}$$

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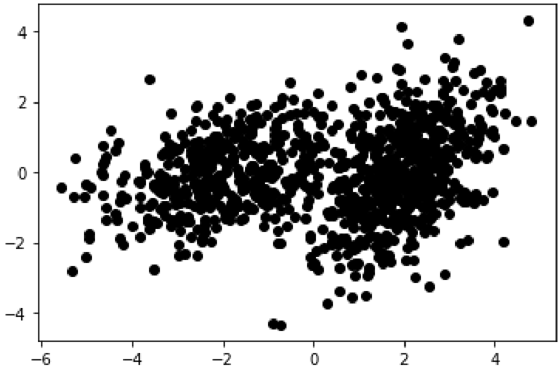
3. Add $\boldsymbol{x}$ to S, go to step 1

Illustration

Here is an example data set S with 1,000 samples



No label information available

The Learning Problem

Consider using the following distribution to fit the data S

$$q(\boldsymbol{x}) = \alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1-\alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \tag{33}$$

The Learning Problem

Consider using the following distribution to fit the data S

$$q(\boldsymbol{x}) = \alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1 - \alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \tag{33}$$

- This is a *density estimation* problem — one of the unsupervised learning problems

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- This is a *density estimation* problem — one of the unsupervised learning problems
- The number of components in $q(\boldsymbol{x})$ is part of the assumption based on *our understanding* about the data
- Without knowing the true data distribution, the number of components is treated as a hyper-parameter (predetermined before learning)

Parameter Estimation

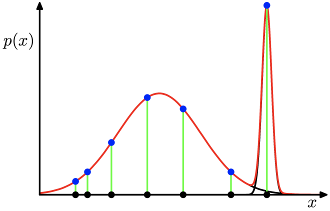
- Based on the general form of GMMs, the parameters are $\boldsymbol{\theta} = \{\alpha, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2\}$
- Given a set of training example $S = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$, the straightforward method is MLE

$$\begin{aligned} L(\boldsymbol{\theta}) &= \sum_{i=1}^{m} \log q(\boldsymbol{x}_i; \boldsymbol{\theta}) \\ &= \sum_{i=1}^{m} \log \Big(\alpha \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ &\quad + (1-\alpha) \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \Big) \end{aligned} \tag{34}$$

- Learning: $\boldsymbol{\theta} \leftarrow \operatorname{argmax}_{\boldsymbol{\theta}'} L(\boldsymbol{\theta}')$

Singularity in GMM Parameter Estimation

Singularity happens when one of the mixture component only captures a single data point, which eventually leads the (log-)likelihood to ∞



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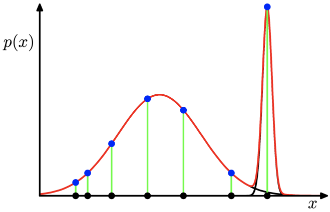

- It is easy to overfit the training set using GMMs, for example when $K = m$

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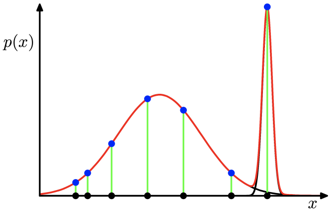

- It is easy to overfit the training set using GMMs, for example when $K = m$
- This issue does not exist when estimating parameters for a single Gaussian distribution

Gradient-based Learning

Recall the definition of $L(\boldsymbol{\theta})$

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{m} \log\left(\alpha \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1-\alpha) \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)\right) \quad (35)$$

- There is no closed form solution of $\nabla L(\boldsymbol{\theta}) = 0$
  - E.g., the value of α depends on $\{\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c\}_{c=1}^{2}$, vice versa
- Gradient-based learning is still *feasible* as

$$\boldsymbol{\theta}^{(\text{new})} \leftarrow \boldsymbol{\theta}^{(\text{old})} + \eta \cdot \nabla L(\boldsymbol{\theta})$$

Latent Variable Models

To rewrite equation 33 into a full probabilistic form, we introduce a random variable $z \in \{1, 2\}$, with

$$q(z = 1) = \alpha \quad q(z = 2) = 1 - \alpha \tag{36}$$

or

$$q(z) = \alpha^{\delta(z=1)}(1 - \alpha)^{\delta(z=2)} \tag{37}$$

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- z is a random variable and indicates the mixture component for $\boldsymbol{x}$ (a similar role as y in the classification problem)
- z is not directly observed in the data, therefore it is a latent (random) variable.

GMM with Latent Variable

With latent variable z, we can rewrite the probabilistic model as a joint distribution over $\boldsymbol{x}$ and z

$$\begin{aligned} q(\boldsymbol{x}, z) &= q(z)q(\boldsymbol{x} \mid z) \\ &= \alpha^{\delta(z=1)} \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)^{\delta(z=1)} \\ &\quad \cdot (1-\alpha)^{\delta(z=2)} \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)^{\delta(z=2)} \end{aligned} \tag{38}$$

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\end{aligned}
$$

And the marginal probability $p(\boldsymbol{x})$ is the same as in equation 33

$$
\begin{aligned}
q(\boldsymbol{x}) &= q(z=1) q(\boldsymbol{x} \mid z=1) + q(z=2) q(\boldsymbol{x} \mid z=2) \\
&= \alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1-\alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \qquad (39)
\end{aligned}
$$

Parameter Estimation: MLE?

For each $\boldsymbol{x}_i$, we introduce a latent variable z_i as mixture component indicator, then the log likelihood is defined as

$$
\begin{aligned}
\ell(\boldsymbol{\theta}) &= \sum_{i=1}^{m} \log q(\boldsymbol{x}_i, z_i) \\
&= \sum_{i=1}^{m} \log \left\{ \alpha^{\delta(z_i=1)} \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)^{\delta(z_i=1)} \right. \\
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&= \sum_{i=1}^{m} \left\{ \delta(z_i = 1) \log \alpha + \delta(z_i = 1) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \right. \\
&\quad \left. \delta(z_i = 2) \log(1-\alpha) + \delta(z_i = 2) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right\}
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&\qquad \left. \delta(z_i = 2) \log(1-\alpha) + \delta(z_i = 2) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right\}
\end{aligned}$$

Question: we have already know that z_i is a random variable, but $E[z_i = 1] = \alpha$?

EM Algorithm

Basic Idea

- The key challenge of GMM with latent variables is that we do not know the distributions of $\{z_i\}$

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- The basic idea of the EM algorithm is to alternatively address the challenge between

$$\{z_i\}_{i=1}^{m} \Leftrightarrow \boldsymbol{\theta} = \{\alpha, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2\} \tag{41}$$

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- The key challenge of GMM with latent variables is that we do not know the distributions of $\{z_i\}$
- The basic idea of the EM algorithm is to alternatively address the challenge between

$$\{z_i\}_{i=1}^m \Leftrightarrow \boldsymbol{\theta} = \{\alpha, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2\} \tag{41}$$

- Basic procedure
  1. Fix $\boldsymbol{\theta}$, estimate the distributions of $\{z_i\}_{i=1}^m$
  2. Fix the distribution of $\{z_i\}_{i=1}^m$, estimate the value of $\boldsymbol{\theta}$
  3. Go back to step 1

How to Estimate z_i?

Fix $\boldsymbol{\theta}$, we can estimate the distribution of each z_i as (with equation 38 and 39)

$$q(z_i \mid \boldsymbol{x}_i) = \frac{q(\boldsymbol{x}_i, z_i)}{q(\boldsymbol{x}_i)} \tag{42}$$

Particularly, we have

$$q(z_i = 1 \mid \boldsymbol{x}_i) = \frac{\alpha \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)}{\alpha \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1 - \alpha) \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)} \tag{43}$$

Expectation

Let γ_i be the expectation of z_i under the distribution of $q(z_i \mid \boldsymbol{x}_i)$

$$E[z_i] = \gamma_i \tag{44}$$

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Expectation

Let γ_i be the expectation of z_i under the distribution of $q(z_i \mid \boldsymbol{x}_i)$

$$E\left[z_i\right] = \gamma_i \tag{44}$$

- Since z_i is a Bernoulli random variable, we also have $q(z_i = 1 \mid \boldsymbol{x}_i) = \gamma_i$
- Furthermore, the expectation of $\delta(z_i = 1)$ under the distribution of $q(z_i \mid \boldsymbol{x}_i)$

$$\begin{aligned} E\left[\delta(z_i = 1)\right] &= \delta(z_i = 1) \cdot q(z_i = 1 \mid \boldsymbol{x}_i) \\ &\quad + \delta(z_i = 1) \cdot q(z_i = 2 \mid \boldsymbol{x}_i) \\ &= q(z_i = 1) = \gamma_i \end{aligned} \tag{45}$$

Parameter Estimation (I)

Given

$$\begin{aligned}\ell(\boldsymbol{\theta}) = \sum_{i=1}^{m} \Big\{ & \delta(z_i = 1) \log \alpha + \delta(z_i = 1) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ & \delta(z_i = 2) \log(1 - \alpha) + \delta(z_i = 2) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \Big\}\end{aligned} \tag{46}$$

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To maximize $\ell(\boldsymbol{\theta})$ with respect to α we have

$$\sum_{i=1}^{m} \left\{ \frac{\delta(z_i = 1)}{\alpha} - \frac{\delta(z_i = 2)}{1 - \alpha} \right\} = 0 \tag{47}$$

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and

$$\alpha \mid \boldsymbol{z} = \frac{\sum_{i=1}^{m} \delta(z_i = 1)}{\sum_{i=1}^{m} (\delta(z_i = 1) + \delta(z_i = 2))} = \frac{\sum_{i=1}^{m} \delta(z_i = 1)}{m} \tag{48}$$

which is similar to the classification example, except that z_i is a *random variable*

Parameter Estimation (II)

Without going through the details, the estimate of *mean* and *covariance* take the similar forms. For example, for the first component, we have

$$\boldsymbol{\mu}_1 \mid \boldsymbol{z} = \frac{1}{m}\sum_{i=1}^{m} \delta(z_i = 1)\boldsymbol{x}_i \tag{49}$$

$$\boldsymbol{\Sigma}_1 \mid \boldsymbol{z} = \frac{1}{m}\sum_{i=1}^{m} \delta(z_i = 1)(\boldsymbol{x}_i - \boldsymbol{\mu}_1)(\boldsymbol{x}_i - \boldsymbol{\mu}_1)^\top \tag{50}$$

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Question: how to eliminate the randomness in α, $\boldsymbol{\mu}_1$, $\boldsymbol{\Sigma}_1$ (and similarly in $\boldsymbol{\mu}_2$, $\boldsymbol{\Sigma}_2$)?

Expectation (II)

With $E[\delta(z_i = 1)] = \gamma_i$, we have

$$\begin{aligned} \alpha &= E[\alpha \mid \boldsymbol{z}] = \frac{1}{m} \sum_{i=1}^{m} E[\delta(z_i = 1)] \boldsymbol{x}_i \\ &= \frac{1}{m} \sum_{i=1}^{m} \gamma_i \boldsymbol{x}_i \end{aligned} \tag{51}$$

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Similarly, we have

$$\boldsymbol{\mu}_1 = \frac{1}{m}\sum_{i=1}^{m} \gamma_i \boldsymbol{x}_i \qquad \boldsymbol{\mu}_2 = \frac{1}{m}\sum_{i=1}^{m} (1-\gamma_i)\boldsymbol{x}_i$$

$$\begin{aligned} \boldsymbol{\Sigma}_1 &= \frac{1}{m}\sum_{i=1}^{m} \gamma_i(\boldsymbol{x}_i - \boldsymbol{\mu}_1)(\boldsymbol{x}_i - \boldsymbol{\mu}_1)^{\mathsf{T}} \\ \boldsymbol{\Sigma}_2 &= \frac{1}{m}\sum_{i=1}^{m} (1-\gamma_i)(\boldsymbol{x}_i - \boldsymbol{\mu}_2)(\boldsymbol{x}_i - \boldsymbol{\mu}_2)^{\mathsf{T}} \end{aligned} \tag{52}$$

The EM Algorithm, Review

The algorithm iteratively run the following two steps:

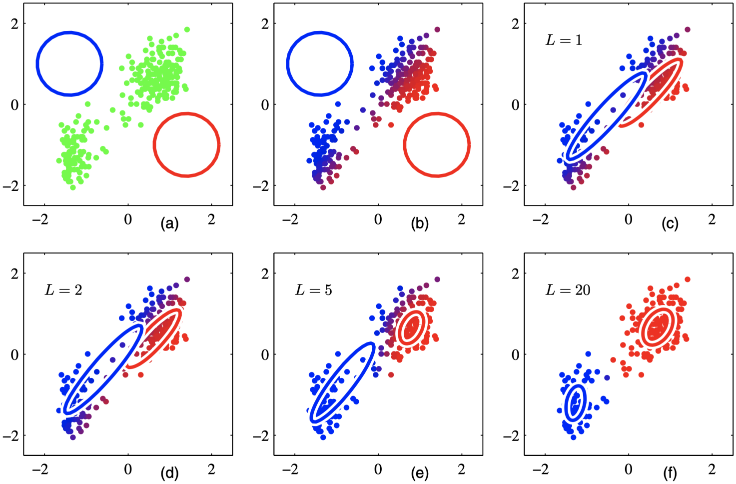
E-step Given $\boldsymbol{\theta}$, for each $\boldsymbol{x}_i$, estimate the distribution of the corresponding latent variable z_i

$$q(z_i \mid \boldsymbol{x}_i) = \frac{q(\boldsymbol{x}_i, z_i)}{q(\boldsymbol{x}_i)} \tag{53}$$

and its expectation γ_i

M-step Given $\{z_i\}_{i=1}^m$, maximize the log-likelihood function $\ell(\boldsymbol{\theta})$ and estimate the parameter $\boldsymbol{\theta}$ with $\{\gamma_i\}_{i=1}^m$

Illustration



[Bishop, 2006, Page 437]

Variational Inference (Optional)

The Computation of $q(z \mid \boldsymbol{x})$

- In the previous example, we were able to compute the analytic solution of $q(z \mid \boldsymbol{x})$ as

$$q(z \mid \boldsymbol{x}) = \frac{q(\boldsymbol{x}, z)}{q(\boldsymbol{x})} \tag{54}$$

where $q(\boldsymbol{x}) = \sum_z q(\boldsymbol{x}, z)$

- **Challenge**: Unlike the simple case in GMMs, usually $q(\boldsymbol{x})$ is difficult to compute

$$\begin{aligned} q(\boldsymbol{x}) &= \sum_z q(\boldsymbol{x}, z) \quad \text{discrete} && (55) \\ &= \int_z q(\boldsymbol{x}, z) dz \quad \text{continuous} && (56) \end{aligned}$$

Solution

- Instead of computing $q(\boldsymbol{x})$ and then $q(z \mid \boldsymbol{x})$, we propose another distribution $q'(z \mid \boldsymbol{x})$ to approximate $q(z \mid \boldsymbol{x})$

$$q'(z \mid \boldsymbol{x}) \approx q(z \mid \boldsymbol{x}) \tag{57}$$

  where $q'(z \mid \boldsymbol{x})$ should be *simple* enough to facilitate the computation

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$$q'(z \mid \boldsymbol{x}) \approx q(z \mid \boldsymbol{x}) \tag{57}$$

  where $q'(z \mid \boldsymbol{x})$ should be *simple* enough to facilitate the computation
- The objective of finding a good approximation is the Kullback–Leibler (KL) divergence

$$\begin{aligned} \mathrm{KL}(q' \| q) &= \sum_{z} q'(z \mid \boldsymbol{x}) \log \frac{q'(z \mid \boldsymbol{x})}{q(z \mid \boldsymbol{x})} \quad \text{discrete} \\ &= \int_{z} q'(z \mid \boldsymbol{x}) \log \frac{q'(z \mid \boldsymbol{x})}{q(z \mid \boldsymbol{x})} dz \quad \text{continuous} \end{aligned}$$

KL Divergence

- $\mathrm{KL}(q' \| q) \geq 0$ and the equality holds if and only if $q' = q$

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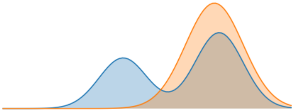
- Regardless what $q(z \mid \boldsymbol{x})$ looks like, we decide to define $q'(z \mid \boldsymbol{x})$ for simplicity



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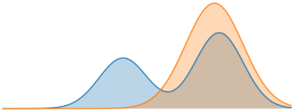

- Because of $q(z \mid \boldsymbol{x})$ in equation 58, the challenge still exists

ELBo

The learning objective for $q'(z \mid \boldsymbol{x})$ is

$$\mathrm{KL}(q' \| q) = \int_z q'(z \mid \boldsymbol{x}) \log \frac{q'(z \mid \boldsymbol{x})}{q(z \mid \boldsymbol{x})} dz$$

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&= \int_z q'(z \mid \boldsymbol{x}) \log \frac{q'(z \mid \boldsymbol{x}) q(\boldsymbol{x})}{q(\boldsymbol{x} \mid z) q(z)} dz
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&= \int_z q'(z \mid \boldsymbol{x}) \left\{ -\log q(\boldsymbol{x} \mid z) + \log \frac{q'(z \mid \boldsymbol{x})}{q(z)} + \log q(\boldsymbol{x}) \right\} dz \\
&= -E\left[\log q(\boldsymbol{x} \mid z)\right] + \mathrm{KL}(q'(z \mid \boldsymbol{x}) \| q(z)) + \log q(\boldsymbol{x})
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&= -E\left[\log q(\boldsymbol{x} \mid z)\right] + \mathrm{KL}(q'(z \mid \boldsymbol{x}) \| q(z)) + \log q(\boldsymbol{x}) \\
&= -\mathrm{ELBo} + \log q(\boldsymbol{x})
\end{aligned}$$

Minimize $\mathrm{KL}(q' \| q)$ is equivalent to maximize the Evidence Lower Bound (ELBo)

Reference

Bishop, C. M. (2006).
Pattern recognition and machine learning.
springer.