

CS 6316 Machine Learning

Generative Models

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ENGINEERING

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 $x \in \mathcal{X}$ according to \mathcal{D}
3. annotate it using the labeling function f as $y = f(x)$

[From Lecture 02]

Example

Here is an data generation model

$$p(x) = \underbrace{0.6 \cdot \mathcal{N}(x; \mu_+, \Sigma_+)}_{y=+1} + \underbrace{0.4 \cdot \mathcal{N}(x; \mu_-, \Sigma_-)}_{y=-1} \quad (1)$$

with

- ▶ $\mu_+ = [2, 0]^T$
- ▶ $\Sigma_+ = \begin{bmatrix} 1.0 & 0.8 \\ 0.8 & 2.0 \end{bmatrix}$
- ▶ $\mu_- = [-2, 0]^T$
- ▶ $\Sigma_- = \begin{bmatrix} 2.0 & 0.6 \\ 0.6 & 1.0 \end{bmatrix}$

Example (II)

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

$$p(y = +1) = 0.6 \quad (2)$$

$$p(y = -1) = 1 - p(y = +1) = 0.4 \quad (3)$$

$$p(\mathbf{x} \mid y = +1) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_+, \boldsymbol{\Sigma}_+) \quad (4)$$

$$p(\mathbf{x} \mid y = -1) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_-, \boldsymbol{\Sigma}_-) \quad (5)$$

Data Generation

The specific data generation process:
for each data point

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

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

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$$p(x | y) = \begin{cases} \mathcal{N}(x; \mu_+, \Sigma_+) & y = +1 \\ \mathcal{N}(x; \mu_-, \Sigma_-) & y = -1 \end{cases} \quad (7)$$

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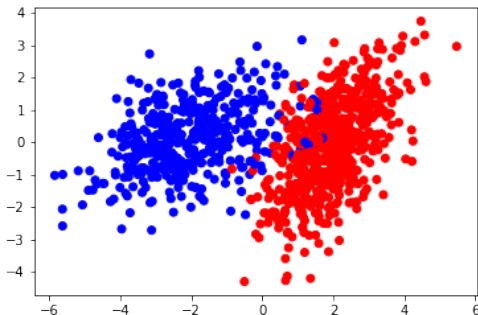
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3. Add (x, y) to S , go to step 1

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

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

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

Generative Models for Classification

- ▶ Basic idea: Building a classifier by *simulating* the data generation process

Generative Models for Classification

- ▶ Basic idea: Building a classifier by *simulating* the data generation process
- ▶ For the binary classification problem, recall the basic components of the data generation process
 - ▶ $p(y)$ where $y \in \{-1, +1\}$
 - ▶ $p(x \mid y = +1)$ where $x \in \mathbb{R}^d$
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 - ▶ $p(x \mid y = +1)$ where $x \in \mathbb{R}^d$
 - ▶ $p(x \mid y = -1)$ where $x \in \mathbb{R}^d$
- ▶ 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
$p(y)$	$q(y)$
$p(x \mid y = +1)$	$q(x \mid y = +1)$
$p(x \mid y = -1)$	$q(x \mid y = -1)$

Learning with Generative Models

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

Defining Distributions

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- ▶ Similarly, for $p(x \mid y = -1)$

$$p(x \mid y = -1) = \mathcal{N}(x; \mu_-, \Sigma_-) \quad (11)$$

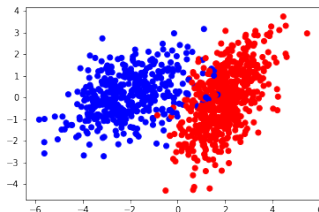
where μ_- and Σ_- are the parameters

Parameter Estimation

- ▶ The collection of the parameters

$$\theta = \{\alpha, \mu_+, \Sigma_+, \mu_-, \Sigma_-\} \quad (12)$$

- ▶ Training data $S = \{(x_1, y_1), \dots, (x_m, y_m)\}$

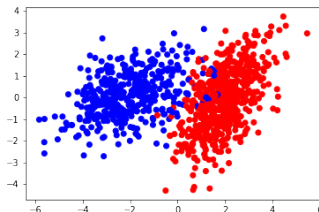


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- ▶ Learning algorithm: Maximum Likelihood Estimation (MLE)

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MLE defined on the whole distribution $q(x, y)$

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Based on the chain rule of probability

$$q(x, y; \theta) = q(y; \alpha)q(x \mid y; \mu_y, \Sigma_y), \quad (14)$$

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Therefore

$$\hat{\theta} \leftarrow \operatorname{argmax}_{\theta} \left\{ \sum_{i=1}^m \log q(y_i; \alpha) + \sum_{i=1}^m \log q(x_i \mid y_i; \mu_y, \Sigma_y) \right\}$$

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

MLE: Bernoulli Distribution

Recall the definition of Bernoulli distribution, we have

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

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Then, the value of α can be estimated from

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

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therefore,

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

MLE: Gaussian Distribution

The definition of multi-variate Gaussian distribution

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

- For $y = +1$, MLE on μ_+ and Σ_+ will only consider the samples x with $y = +1$ (assume it's S_+)

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- ▶ MLE on μ_+

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

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

Example: Parameter Estimation

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

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

Prediction

- ▶ For a new data point x' , the prediction is given as

$$q(y' | x') = \frac{q(y')q(x | y')}{q(x')} \propto q(y')q(x' | y') \quad (21)$$

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

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No need to compute $q(\mathbf{x}')$

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

$$q(y' | \mathbf{x}') \approx p(y | \mathbf{x}) \quad (23)$$

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

Naive Bayes Classifiers

Number of Parameters

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

- ▶ $q(y)$: 1 (α)
- ▶ $q(\mathbf{x} \mid y = +1)$:
 - ▶ $\mu_+ \in \mathbb{R}^d$: d parameters
 - ▶ $\Sigma_+ \in \mathbb{R}^{d \times d}$: d^2 parameters
- ▶ $q(\mathbf{x} \mid y = -1)$: $d^2 + d$ 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 Σ in a multivariate Gaussian distribution

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

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- ▶ To reduce the number of parameters, we assume

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

Diagonal Covariance Matrix

With the diagonal covariance matrix

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

Now, the multivariate Gaussian distribution can be rewritten with

$$|\Sigma| = \prod_{j=1}^d \sigma_{j,j}^2 \quad (27)$$

$$(x - \mu)^\top \Sigma^{-1} (x - \mu) = \sum_{j=1}^d \frac{(x_{\cdot,j} - \mu_j)^2}{\sigma_{j,j}^2} \quad (28)$$

Diagonal Covariance Matrix (II)

In other words

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

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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

$$p(x) = \underbrace{\alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1)}_{c=1} + \underbrace{(1 - \alpha) \cdot \mathcal{N}(x; \mu_2, \Sigma_2)}_{c=2} \quad (30)$$

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- ▶ No labeling information
- ▶ 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

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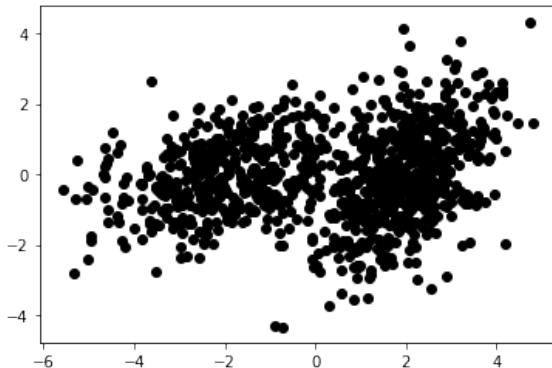
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3. Add x to S , go to step 1

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

$$q(x) = \alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1) + (1 - \alpha) \cdot \mathcal{N}(x; \mu_2, \Sigma_2) \quad (33)$$

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- ▶ This is a *density estimation* problem — one of the unsupervised learning problems
- ▶ The number of components in $q(x)$ 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

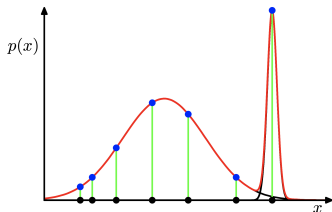
- ▶ Based on the general form of GMMs, the parameters are $\theta = \{\alpha, \mu_1, \Sigma_1, \mu_2, \Sigma_2\}$
- ▶ Given a set of training example $S = \{x_1, \dots, x_m\}$, the straightforward method is MLE

$$\begin{aligned} L(\theta) &= \sum_{i=1}^m \log q(x_i; \theta) \\ &= \sum_{i=1}^m \log \left(\alpha \cdot \mathcal{N}(x_i; \mu_1, \Sigma_1) \right. \\ &\quad \left. + (1 - \alpha) \cdot \mathcal{N}(x_i; \mu_2, \Sigma_2) \right) \end{aligned} \quad (34)$$

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

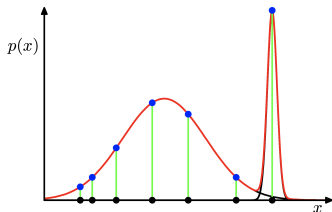
Singularity in GMM Parameter Estimation

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



Singularity in GMM Parameter Estimation

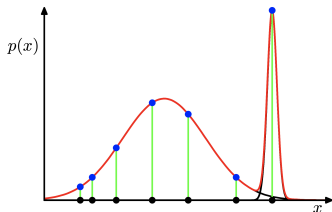
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Singularity in GMM Parameter Estimation

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



- ▶ 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 $L(\boldsymbol{\theta})$

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

- ▶ 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

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

or

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

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- ▶ z is a random variable and indicates the mixture component for 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 x and z

$$\begin{aligned} q(x, z) &= q(z)q(x | z) \\ &= \alpha^{\delta(z=1)} \cdot \mathcal{N}(x; \mu_1, \Sigma_1)^{\delta(z=1)} \\ &\quad \cdot (1 - \alpha)^{\delta(z=2)} \cdot \mathcal{N}(x; \mu_2, \Sigma_2)^{\delta(z=2)} \end{aligned} \quad (38)$$

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And the marginal probability $p(x)$ is the same as in equation 33

$$\begin{aligned} q(x) &= q(z = 1)q(x | z = 1) + q(z = 2)q(x | z = 2) \\ &= \alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1) + (1 - \alpha) \cdot \mathcal{N}(x; \mu_2, \Sigma_2) \end{aligned} \quad (39)$$

Parameter Estimation: MLE?

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

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= \sum_{i=1}^m \log q(\mathbf{x}_i, z_i) \\ &= \sum_{i=1}^m \log \left\{ \alpha^{\delta(z_i=1)} \cdot \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)^{\delta(z_i=1)} \right. \\ &\quad \left. \cdot (1 - \alpha)^{\delta(z_i=2)} \cdot \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)^{\delta(z_i=2)} \right\} \\ &= \sum_{i=1}^m \left\{ \delta(z_i = 1) \log \alpha + \delta(z_i = 1) \log \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \right. \\ &\quad \left. \delta(z_i = 2) \log(1 - \alpha) + \delta(z_i = 2) \log \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right\}\end{aligned}\tag{40}$$

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

EM Algorithm

Basic Idea

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

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

How to Estimate z_i ?

Fix θ , we can estimate the distribution of each z_i as (with equation 38 and 39)

$$q(z_i \mid \mathbf{x}_i) = \frac{q(\mathbf{x}_i, z_i)}{q(\mathbf{x}_i)} \quad (42)$$

Particularly, we have

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

Expectation

Let γ_i be the **expectation** of z_i

$$E[z_i] = \gamma_i \quad (44)$$

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Expectation

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- ▶ Since z_i is a Bernoulli random variable, we also have

$$p(z_i = 1) = \gamma_i$$

- ▶ Furthermore, the expectation of $\delta(z_i = 1)$

$$\begin{aligned} E[\delta(z_i = 1)] &= \delta(z_i = 1) \cdot p(z_i = 1) + \delta(z_i = 1) \cdot p(z_i = 2) \\ &= p(z_i = 1) = \gamma_i \end{aligned} \quad (45)$$

Parameter Estimation (I)

Given

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^m \left\{ \delta(z_i = 1) \log \alpha + \delta(z_i = 1) \log \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \right. \\ \left. \delta(z_i = 2) \log(1 - \alpha) + \delta(z_i = 2) \log \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right\} \quad (46)$$

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

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

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

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

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

and

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

which is similar to the classification example, except 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

$$\mu_1 | z = \frac{1}{m} \sum_{i=1}^m \delta(z_i = 1) x_i \quad (49)$$

$$\Sigma_1 | z = \frac{1}{m} \sum_{i=1}^m \delta(z_i = 1) (x_i - \mu_1)(x_i - \mu_1)^\top \quad (50)$$

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Question: how to eliminate the randomness in α, μ_1, Σ_1 (and similarly in μ_2, Σ_2)?

Expectation (II)

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

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

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Similarly, we have

$$\begin{aligned}\mu_1 &= \frac{1}{m} \sum_{i=1}^m \gamma_i \mathbf{x}_i & \mu_2 &= \frac{1}{m} \sum_{i=1}^m (1 - \gamma_i) \mathbf{x}_i \\ \Sigma_1 &= \frac{1}{m} \sum_{i=1}^m \gamma_i (\mathbf{x}_i - \mu_1)(\mathbf{x}_i - \mu_1)^\top \\ \Sigma_2 &= \frac{1}{m} \sum_{i=1}^m (1 - \gamma_i) (\mathbf{x}_i - \mu_2)(\mathbf{x}_i - \mu_2)^\top\end{aligned}\tag{52}$$

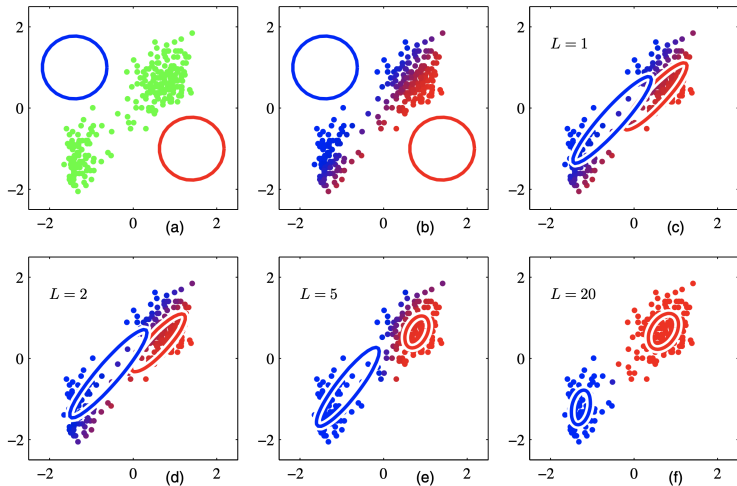
The EM Algorithm, review

The algorithm iteratively run the following two steps:

E-step Given θ , for each x_i , estimate the distribution of the corresponding latent variable z_i and its **expectation** γ_i

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

Illustration



[?, Page 437]

Reference