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 \mathfrak{X} , label set \mathfrak{Y} , and the training set S

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

[From Lecture 02]

Example

Here is an data generation model

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

with

$$\mu_+ = [2, 0]^T$$

$$\Sigma_{+} = \left[\begin{array}{cc} 1.0 & 0.8 \\ 0.8 & 2.0 \end{array} \right]$$

$$\mu_{-} = [-2, 0]^{\mathsf{T}}$$

$$\Sigma_{-} = \begin{bmatrix} 2.0 & 0.6 \\ 0.6 & 1.0 \end{bmatrix}$$

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Example (II)

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

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

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

$$p(x \mid y = +1) = \mathcal{N}(x; \mu_+, \Sigma_+) \tag{4}$$

$$p(x \mid y = -1) = \mathcal{N}(x; \mu_{-}, \Sigma_{-})$$
 (5)

4

Data Generation

The specific data generation process: for each data point

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

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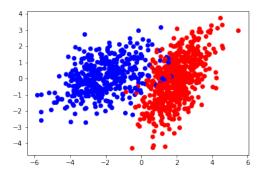
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 (7)

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

$$p(y \mid x) = \sigma(y\langle w, x \rangle) = \frac{1}{1 + e^{-y\langle w, x \rangle}}$$
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- Other examples
 - ► AdaBoost (lecture o5)
 - SVMs (lecture 07)
 - ► Feed-forward neural network (lecture o8)

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- 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 $x \in \mathbb{R}^d$
 - ▶ $p(x \mid y = -1)$ where $x \in \mathbb{R}^d$

Generative Models for Classification

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

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

$$p(y) = \operatorname{Bern}(y; \alpha) = \alpha^{\delta(y=+1)} (1 - \alpha)^{\delta(y=-1)}$$
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► Similarly, for $p(x \mid y = -1)$

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

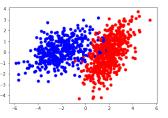
where μ_{-} and Σ_{-} are the parameters

Parameter Estimation

► The collection of the parameters

$$\theta = \{\alpha, \mu_+, \Sigma_+, \mu_-, \Sigma_-\} \tag{12}$$

► Training data $S = \{(x_1, y_1), ..., (x_m, y_m)\}$

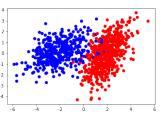


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 Learning algorithm: Maximum Likelihood Estimation (MLE)

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

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Based on the chain rule of probability

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

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

Therefore

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

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

MLE: Bernoulli Distribution

Recall the definition of Bernoulli distribution, we have

$$\sum_{i=1}^{m} \log q(y_i; \alpha) = \sum_{i=1}^{m} \{ \delta(y_i = +1) \log \alpha + \delta(y_i = -1) \log(1 - \alpha) \}$$
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Then, the value of α can be estimated from

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

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

The definition of multi-variate Gaussian distribution

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

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- ▶ MLE on μ_+

$$\mu = \frac{1}{|S_+|} \sum_{x_i \in S_+} x_i \tag{19}$$

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 (20)

• Exercise: prove equations 19 and 20 with d = 1

Example: Parameter Estimation

Given N = 1000 samples, here are the parameters

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

Prediction

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

$$q(y' \mid x') = \frac{q(y')q(x \mid y')}{q(x')} \propto q(y')q(x' \mid y')$$
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$$y' = \begin{cases} +1 & q(y' = +1 \mid x') > q(y' = -1 \mid x') \\ -1 & q(y' = +1 \mid x') < q(y' = +1 \mid x') \end{cases}$$
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Although equation 22 looks like the one used in the Bayes optimal predictor, the prediction power is limited by

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

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

Naive Bayes Classifiers

Number of Parameters

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

- ightharpoonup q(y): 1 (α)
- $q(x \mid y = +1):$
 - ▶ μ_+ ∈ \mathbb{R}^d : d parameters
 - $\Sigma_+ \in \mathbb{R}^{d \times d}$: d^2 parameters
- $q(x \mid y = -1)$: $d^2 + d$ 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

$$\Sigma = \begin{bmatrix} \sigma_{1,1}^2 & \cdots & \sigma_{1,d}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{d,1}^2 & \cdots & \sigma_{d,d}^2 \end{bmatrix}$$
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► To reduce the number of parameters, we assume

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

With the diagonal covariance matrix

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

Now, the multivariate Gaussian distribution can be rewritten with

- $\blacktriangleright |\Sigma| = \prod_{j=1}^d \sigma_{j,j}^2$
- assume $\mu = 0$ for simplicity

$$(x - \mu)^{\mathsf{T}} \Sigma^{-1} (x - \mu) = \sum_{j=1}^{d} \frac{(x_{\cdot,j} - \mu_j)^2}{\sigma_{j,j}^2}$$
 (27)

$$q(x \mid y, \mu, \Sigma) = \prod_{j=1}^{d} q(x_{\cdot,j} \mid y; \mu_j, \sigma_{j,j}^2)$$
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In other words

$$q(x \mid y, \mu, \Sigma) = \prod_{j=1}^{d} q(x_{,j} \mid y; \mu_{j}, \sigma_{j,j}^{2})$$
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- Parameter estimation can be done per dimension

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Data Generation Model, Revisited

Consider the following model again without any label information

$$p(x) = \underbrace{\alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)}_{c=1} + \underbrace{(1 - \alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)}_{c=2}$$
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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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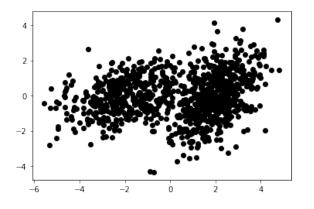
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3. Add x to S, go to step 1

Illustration

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



No label information available

Consider using the following distribution to fit the data *S*

$$q(x) = \alpha \cdot \mathcal{N}(x; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1 - \alpha) \cdot \mathcal{N}(x; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$
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- ► The number of components in q(x) is part of the assumption based on *our understanding* about the data

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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 $S = \{x_1, ..., x_m\}$, the straightforward method is MLE

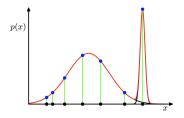
$$L(\theta) = \sum_{i=1}^{m} \log q(x_i; \theta)$$

$$= \sum_{i=1}^{m} \log \left(\alpha \cdot \mathcal{N}(x_i; \mu_1, \Sigma_1) + (1 - \alpha) \cdot \mathcal{N}(x_i; \mu_2, \Sigma_2)\right)$$
(33)

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

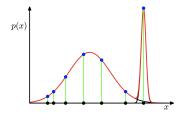
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Singularity happens when one of the mixture component only captures a single data point, which eventually leads the (log-)likelihood to ∞



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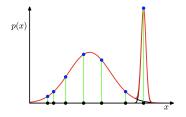
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► It is easy to overfit the training set using GMMs, for example when K = m

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 $L(\theta)$

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{m} \log \left(\alpha \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + (1 - \alpha) \cdot \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right)$$
(34)

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

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

To rewrite equation 32 into a full probabilistic form, we introduce a random variable $z \in \{1, 2\}$, with

$$q(z = 1) = \alpha \quad q(z = 2) = 1 - \alpha$$
 (35)

or

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

$$q(x,z) = q(z)q(x \mid z)$$

$$= \alpha^{\delta(z=1)} \cdot \mathcal{N}(x; \mu_1, \Sigma_1)^{\delta(z=1)}$$

$$\cdot (1-\alpha)^{\delta(z=2)} \cdot \mathcal{N}(x; \mu_2, \Sigma_2)^{\delta(z=2)}$$
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And the marginal probability p(x) is the same as in equation 32

$$q(x) = q(z = 1)q(x \mid z = 1) + q(z = 2)q(x \mid z = 2)$$

= $\alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1) + (1 - \alpha) \cdot \mathcal{N}(x; \mu_2, \Sigma_2)$ (38)

Parameter Estimation: MLE?

For each x_i , we introduce a latent variable z_i as mixture component indictor, then the log likelihood is defined as

$$\ell(\theta) = \sum_{i=1}^{m} \log q(x_i, z_i)$$

$$= \sum_{i=1}^{m} \log \left\{ \alpha^{\delta(z_i=1)} \cdot \mathcal{N}(x_i; \mu_1, \Sigma_1)^{\delta(z_i=1)} \right.$$

$$\cdot (1 - \alpha)^{\delta(z_i=2)} \cdot \mathcal{N}(x_i; \mu_2, \Sigma_2)^{\delta(z_i=2)} \right\}$$

$$= \sum_{i=1}^{m} \left\{ \delta(z_i = 1) \log \alpha + \delta(z_i = 1) \log \mathcal{N}(x_i; \mu_1, \Sigma_1) \right.$$

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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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 (40)

- 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 37 and 38)

$$q(z_i \mid x_i) = \frac{q(x_i, z_i)}{q(x_i)}$$
(41)

Particularly, we have

$$q(z_i = 1 \mid x_i) = \frac{\alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1)}{\alpha \cdot \mathcal{N}(x; \mu_1, \Sigma_1) + (1 - \alpha) \cdot \mathcal{N}(x; \mu_2, \Sigma_2)}$$
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Expactation

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Expactation

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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 $\delta(z_i = 1)$

$$E[\delta(z_i = 1)] = \delta(z_i = 1) \cdot p(z_i = 1) + \delta(z_i = 1) \cdot p(z_i = 2)$$

= $p(z_i = 1) = \gamma_i$ (44)

Parameter Estimation (I)

Given

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

$$\delta(z_i = 2) \log(1 - \alpha) + \delta(z_i = 2) \log \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \right\}$$
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To maximize $\ell(\theta)$ with respect to α we have

$$\sum_{i=1}^{m} \left\{ \frac{\delta(z_i = 1)}{\alpha} - \frac{\delta(z_i = 2)}{1 - \alpha} \right\} = 0$$
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To maximize $\ell(\theta)$ with respect to α we have

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and

$$\alpha \mid \mathbf{z} = \frac{\sum_{i=1}^{m} \delta(z_i = 1)}{\sum_{i=1}^{m} (\delta(z_i = 1) + \delta(z_i = 2))} = \frac{\sum_{i=1}^{m} \delta(z_i = 1)}{m}$$
(47)

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

$$\mu_1 \mid z = \frac{1}{m} \sum_{i=1}^{m} \delta(z_i = 1) x_i$$
 (48)

$$\Sigma_1 \mid z = \frac{1}{m} \sum_{i=1}^m \delta(z_i = 1) (x_i - \mu_1) (x_i - \mu_1)^{\mathsf{T}}$$
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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

$$\alpha = E[\alpha \mid z] = \sum_{i=1}^{m} \frac{1}{m} E[\delta(z_i = 1)] x_i$$

$$= \sum_{i=1}^{m} \gamma_i x_i$$
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(50)

Similarly, we have

$$\mu_{1} = \frac{1}{m} \sum_{i=1}^{m} \gamma_{i} x_{i} \qquad \mu_{2} = \frac{1}{m} \sum_{i=1}^{m} (1 - \gamma_{i}) x_{i}$$

$$\Sigma_{1} = \frac{1}{m} \sum_{i=1}^{m} \gamma_{i} (x_{i} - \mu_{1}) (x_{i} - \mu_{1})^{\mathsf{T}}$$

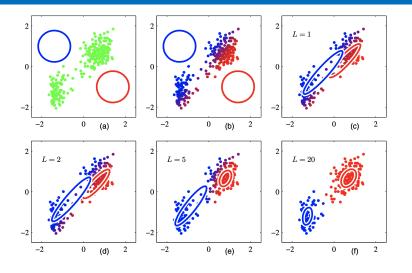
$$\Sigma_{2} = \frac{1}{m} \sum_{i=1}^{m} (1 - \gamma_{i}) (x_{i} - \mu_{2}) (x_{i} - \mu_{2})^{\mathsf{T}} \quad (51)$$

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



[Bishop, 2006, Page 437]

Reference



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