# Lecture 5: Gaussian Discriminant Analysis, Naive Bayes and EM Algorithm 

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## Outline

(1) Probability Theory Review
(2) A Warm-Up Case
(3) Gaussian Discriminate Analysis
(4) Naive Bayes
(5) Expectation-Maximization (EM) Algorithm

## Probability Theory Review

- Sample space, events and probability
- Conditional probability
- Random variables and probability distributions
- Joint probability distribution
- Independence
- Conditional probability distribution
- Bayes' Theorem


## Sample Space, Events and Probability

- A sample space $\mathcal{S}$ is the set of all possible outcomes of a (conceptual or physical) random experiment
- Event A is a subset of the sample space $\mathcal{S}$
- $P(A)$ is the probability that event $A$ happens
- It is a function that maps the event $A$ onto the interval $[0,1]$.
- $P(A)$ is also called the probability measure of $A$
- Kolmogorov axioms
- Non-negativity: $p(A) \geq 0$ for each event $A$
- $P(\mathcal{S})=1$
- $\sigma$-additivity: For disjoint events $\left\{A_{i}\right\}_{i}$ such that $A_{i} \bigcap A_{j}=\emptyset$ for $\forall i \neq j$

$$
P\left(\bigcup_{i=1}^{\infty} A_{i}\right)=\sum_{i=1}^{\infty} P\left(A_{i}\right)
$$

## Sample Space, Events and Probability (Contd.)

- Some consequences
- $P(\emptyset)=0$
- $P(A \bigcup B)=P(A)+P(B)-P(A \bigcap B)$
- $P(A\urcorner)=1-P(A)$


## Conditional Probability

- Definition of conditional probability: Fraction of worlds in which event $A$ is true given event $B$ is true

$$
P(A \mid B)=\frac{P(A, B)}{P(B)}, \quad P(A, B)=P(A \mid B) P(B)
$$

- Corollary: The chain rule

$$
P\left(A_{1}, A_{2}, \cdots, A_{k}\right)=\prod_{k=1}^{n} P\left(A_{k} \mid A_{1}, A_{2}, \cdots, A_{k-1}\right)
$$

- Example:
$P\left(A_{4}, A_{3}, A_{2}, A_{1}\right)=P\left(A_{4} \mid A_{3}, A_{2}, A_{1}\right) P\left(A_{3} \mid A_{2}, A_{1}\right) P\left(A_{2} \mid A_{1}\right) P\left(A_{1}\right)$


## Conditional Probability (Contd.)

- Real valued random variable is a function of the outcome of a randomized experiment

$$
X: \mathcal{S} \rightarrow R
$$

- Examples: Discrete random variables ( $\mathcal{S}$ is discrete)
- $X(s)=$ True if a randomly drawn person $(s)$ from our class $(\mathcal{S})$ is female
- $X(s)=$ The hometown $X(s)$ of a randomly drawn person $(s)$ from $(\mathcal{S})$
- Examples: Continuous random variables ( $\mathcal{S}$ is continuous)
- $X(s)=r$ be the heart rate of a randomly drawn person $s$ in our class $\mathcal{S}$


## Random Variables

- Real valued random variable is a function of the outcome of a randomized experiment

$$
X: \mathcal{S} \rightarrow R
$$

- For continuous random variable $X$

$$
P(a<X<b)=P(\{s \in \mathcal{S}: a<X(s)<b\})
$$

- For discrete random variable $X$

$$
P(X=x)=P(\{s \in \mathcal{S}: X(s)=x\})
$$

## Probability Distribution

- Probability distribution for discrete random variables
- Suppose $X$ is a discrete random variable

$$
x: \mathcal{S} \rightarrow \mathcal{A}
$$

- Probability mass function (PMF) of $X$ : the probability of $X=x$

$$
p_{X}(x)=P(X=x)
$$

- Since $\sum_{x \in \mathcal{A}} P(X=x)=1$, we have

$$
\sum_{x \in \mathcal{A}} p_{X}(x)=1
$$

## Probability Distribution (Contd.)

- Probability distribution for continuous random variables
- Suppose $X$ is a continuous random variable

$$
X: \mathcal{S} \rightarrow \mathcal{A}
$$

- Probability density function (PDF) of $X$ is a function $f_{X}(x)$ such that for $\forall a, b \in \mathcal{A}$ with $(a \leq b)$

$$
P(a \leq X \leq b)=\int_{a}^{b} f_{X}(x) d x
$$

## Joint Probability Distribution

- Joint probability distribution
- Suppose both $X$ and $Y$ are discrete random variable
- Joint probability mass function (PMF)

$$
p_{X, Y}(x, y)=P(X=x, Y=y)
$$

- Marginal probability mass function for discrete random variables

$$
\begin{aligned}
& p_{X}(x)=\sum_{y} P(X=x, Y=y)=\sum_{y} P(X=x \mid Y=y) P(Y=y) \\
& p_{Y}(y)=\sum_{x} P(X=x, Y=y)=\sum_{x} P(Y=y \mid X=x) P(Y=x)
\end{aligned}
$$

- Extension to multiple random variables $X_{1}, X_{2}, X_{3}, \cdots, X_{n}$

$$
p_{X}\left(x_{1}, x_{2}, \cdots, x_{n}\right)=P\left(X_{1}=x_{1}, X_{2}=x_{2}, \cdots, X_{n}=x_{n}\right)
$$

## Joint Probability Distribution (Contd.)

- Joint probability distribution
- Suppose both $X$ and $Y$ are continuous random variable
- Joint probability density function (PDF) $f(x, y)$

$$
P\left(a_{1} \leq X \leq b_{1}, a_{2} \leq Y \leq b_{2}\right)=\int_{a_{1}}^{b_{1}} \int_{a_{2}}^{b_{2}} f(x, y) d x d y
$$

- Marginal probability density functions

$$
\begin{aligned}
& f_{X}(x)=\int_{-\infty}^{\infty} f(x, y) d y \text { for }-\infty<x<\infty \\
& f_{Y}(x)=\int_{-\infty}^{\infty} f(x, y) d x \text { for }-\infty<y<\infty
\end{aligned}
$$

- Extension to more than two random variables

$$
P\left(a_{1} \leq X_{1} \leq b_{1}, \cdots, a_{n} \leq X_{n} \leq b_{n}\right)=\int_{a_{1}}^{b_{1}} \cdots \int_{a_{n}}^{b_{n}} f\left(x_{1}, \cdots, x_{n}\right) d x_{1} \cdots d x
$$

## Independent Random Variables

- Two discrete random variables $X$ and $Y$ are independent if for any pair of $x$ and $y$

$$
p_{X, Y}(x, y)=p_{X}(x) p_{Y}(y)
$$

- Two continuous random variables $X$ and $Y$ are independent if for any pair of $x$ and $y$

$$
f_{X, Y}(x, y)=f_{X}(x) f_{Y}(y)
$$

- If the above equations do not hold for all $(x, y)$, then $X$ and $Y$ are said to be dependent


## Conditional Probability Distribution

- Discrete random variables $X$ and $Y$
- Joint PMF $p(x, y)$
- Marginal PMF $p_{X}(x)=\sum_{y} p(x, y)$
- The Conditional probability density function of $Y$ given $X=x$

$$
p_{Y \mid X}(y \mid x)=\frac{p(x, y)}{p_{X}(x)}, \quad \forall y
$$

or

$$
p_{Y \mid X=x}(y)=\frac{p(x, y)}{p_{X}(x)}, \quad \forall y
$$

- Conditional probability of $Y=y$ given $X=x$

$$
P_{Y=y \mid X=x}=p_{Y \mid X}(y \mid x)
$$

## Conditional Probability Distribution (Contd.)

- Continuous random variables $X$ and $Y$
- Joint PDF $f(x, y)$
- Marginal PDF $f_{X}(x)=\int_{y} f(x, y) d y$
- The Conditional probability density function of $Y$ given $X=x$

$$
f_{Y \mid X}(y \mid x)=\frac{f(x, y)}{f_{X}(x)}, \quad \forall y
$$

or

$$
f_{Y \mid X=x}(y)=\frac{f(x, y)}{f_{X}(x)}, \quad \forall y
$$

- Probability of $a \leq X \leq b$ given $Y=y$

$$
P\left(a_{1} \leq X \leq b_{1} \mid Y=y\right)=\int_{a}^{b} f_{X \mid Y=y}(x) d x
$$

## Conditional Probability Distribution (Contd.)

- Continuous random variables $X$
- Discrete random variable $Y$
- Joint probability distribution

$$
P(a \leq X \leq b, Y=y)=P(a \leq X \leq b \mid Y=y) P(Y=y)
$$

where

$$
\begin{aligned}
& P(a \leq X \leq b \mid Y=y)=\int_{a}^{b} f_{X \mid Y=y}(x) d x \\
& P(Y=y)=p_{Y}(y)
\end{aligned}
$$

## Bayes' Theorem

- Bayes' theorem (or Bayes' rule) describes the probability of an event, based on prior knowledge of conditions that might be related to the event

$$
P(A \mid B)=\frac{P(B \mid A) P(A)}{P(B)}
$$

- In the Bayesian interpretation, probability measures a "degree of belief", and Bayes' theorem links the degree of belief in a proposition before and after accounting for evidence.
- For proposition $A$ and evidence $B$
- $P(A)$, the prior, is the initial degree of belief in $A$
- $P(A \mid B)$, the posterior, is the degree of belief having accounted for $B$
- Another form:

$$
P(A \mid B)=\frac{P(B \mid A) P(A)}{P(B)}=\frac{P(B \mid A) P(A)}{P(B \mid A) P(A)+P(B \mid A\urcorner) P(A\urcorner)}
$$

with $A\urcorner$ being the complement of $A$

## Bayes' Theorem (Contd.)

- A: you have the flu
- $B$ : you just coughed
- Assume: $P(A)=0.05, P(B \mid A)=0.8$, and $P(B \mid A \neg)=0.2\left(A^{\urcorner}\right.$ denotes of the complement of $A$ )
- Question: $P($ flue $\mid$ cough $)=P(A \mid B)$ ?

$$
\begin{aligned}
P(A \mid B) & =\frac{P(B \mid A) P(A)}{P(B)} \\
& =\frac{P(B \mid A) P(A)}{P(B \mid A) P(A)+P(B \mid A\urcorner) P(A\urcorner)} \\
& =\frac{0.8 * 0.05}{0.8 * 0.05+0.2 * 0.95} \\
& \approx 0.18
\end{aligned}
$$

## Bayes' Theorem (Contd.)

- Random variables $X$ and $Y$, both of which are discrete

$$
P(X=x \mid Y=y)=\frac{P(Y=y \mid X=x) P(X=x)}{P(Y=y)}
$$

- Conditional PMF of $X$ given $Y=y$

$$
p_{X \mid Y=y}(x)=\frac{p_{Y \mid X=x}(y) p_{X}(x)}{p_{Y}(y)}
$$

## Bayes' Theorem (Contd.)

- Continuous random variable $X$ and discrete random variable $Y$

$$
\begin{aligned}
f_{X \mid Y=y}(x) & =\frac{P(Y=y \mid X=x) f_{X}(x)}{P(Y=y)} \\
& =\frac{p_{Y \mid X=x}(y) f_{X}(x)}{p_{Y}(y)}
\end{aligned}
$$

## Bayes' Theorem (Contd.)

- Discrete random variable $X$ and continuous random variable $Y$

$$
P(X=x \mid Y=y)=\frac{f_{Y \mid X=x}(y) P(X=x)}{f_{Y}(y)}
$$

- In another form

$$
p_{X \mid Y=y}(x)=\frac{f_{Y \mid X=x}(y) p(x)}{f_{Y}(y)}
$$

## Bayes' Theorem (Contd.)

- $X$ and $Y$ are both continuous

$$
f_{X \mid Y=y}(x)=\frac{f_{Y \mid X=x}(y) f_{X}(x)}{f_{Y}(y)}
$$

## Prediction Based on Bayes' Theorem

- $X$ is a random variable indicating the feature vector
- $Y$ is a random variable indicating the label
- We perform a trial to obtain a sample $x$ for test, and what is

$$
P(Y=y \mid X=x)=p_{Y \mid X}(y \mid x) ?
$$

## Prediction Based on Bayes' Theorem (Contd.)

- We compute $p_{Y \mid X}(y \mid x)$ based on Bayes' Theorem

$$
p_{Y \mid X}(y \mid x)=\frac{p_{X \mid Y}(x \mid y) p_{Y}(y)}{p_{X}(x)}, \forall y
$$

- We calculate $p_{X \mid Y}(x \mid y)$ for $\forall x, y$ and $p_{Y}(y)$ for $\forall y$ according to the given training data
- Fortunately, we do not have to calculate $p_{X}(x)$, because

$$
\begin{aligned}
\arg \max _{y} p_{Y \mid X}(y \mid x) & =\arg \max _{y} \frac{p_{X \mid Y}(x \mid y) p_{Y}(y)}{p_{X}(x)} \\
& =\arg \max _{y} p_{X \mid Y}(x \mid y) p_{Y}(y)
\end{aligned}
$$

## Warm Up

- The world is probabilistic
- You randomly join SDU
- You randomly choose this class
- You may randomly fail this class


## Warm Up (Contd.)

- Task: Identify if there is a cat in a given image.


## Warm Up (Contd.)

- Images (to be classified or to be used for training) are given randomly
- Some of them may contain a cat
- Some of them may not
- Whether there is a cat is random
- An image is represented by a vector of features
- The feature vectors are random, since the images are randomly given
- Random variable $X$ representing the feature vector (and thus the image)
- The labels are random, since the images are randomly given
- Random variable $Y$ representing the label


## Warm Up (Contd.)

- In linear regression and logistic regression, $x$ and $y$ are linked through (deterministic) hypothesis function

$$
y=h_{\theta}(x)
$$

- How to model the (probabilistic) relationship between feature vector $X$ and label $Y$ ?

$$
P(Y=y \mid X=x)=\frac{P(X=x \mid Y=y) P(Y=y)}{P(X=x)}
$$

## Warm Up (Contd.)

- How to model the (probabilistic) relationship between feature vector $X$ and label $Y$ ?

$$
P(Y=y \mid X=x)=\frac{P(X=x \mid Y=y) P(Y=y)}{P(X=x)}
$$

- $P(Y=y \mid X=x)$ : Given an image $X=x$ (whose feature is $x$ ), what is the probability of $Y=y$ (with $y=1$ denoting there is a cat and $y=0$ denoting there is not)?
- $P(X=x \mid Y=y)$ : Given an image with $Y=y$ (whose label is $y$ ), what is the probability that the image has its feature vector being $X=x$ ?
- $P(Y=y)$ : Given a randomly picked image, what is the probability that the image contains a cat?
- $P(X=x)$ : Given a randomly picked image, what is the probability that the image has its feature vector being $X=x$ ?


## Warm Up (Contd.)

- How to model the (probabilistic) relationship between feature vector $X$ and label $Y$ ?

$$
P(Y=y \mid X=x)=\frac{P(X=x \mid Y=y) P(Y=y)}{P(X=x)}
$$

- To predict $y$, we have to know
- $P(X=x \mid Y=y)$ : Given an image with $Y=y$ (whose label is $y$ ), what is the probability that the image has its feature vector being $X=x$ ?
- $P(Y=y)$ : Given a randomly picked image, what is the probability that the image contains a cat?
- $P(X=x)$ : Given a randomly picked image, what is the probability that the image has its feature vector being $X=x$ ?


## Warm Up (Contd.)

- In our case
- If $P(Y=1 \mid X=x) \geq P(Y=0 \mid X=x)$, we conclude that there is a cat
- If $P(Y=0 \mid X=x) \geq P(Y=1 \mid X=x)$, we conclude there is not a cat
- How to compare $P(Y=0 \mid X=x)$ and $P(Y=1 \mid X=x)$

$$
\begin{aligned}
& P(Y=0 \mid X=x)=\frac{P(X=x \mid Y=0) P(Y=0)}{P(X=x)} \\
& P(Y=1 \mid X=x)=\frac{P(X=x \mid Y=1) P(Y=1)}{P(X=x)}
\end{aligned}
$$

- We do not need to know $P(X=x)$


## Warm Up (Contd.)

- We make classification according to

$$
P(Y=y \mid X=x)=\frac{P(X=x \mid Y=y) P(Y=y)}{P(X=x)}
$$

- To make classification, we have to know the following parameters

$$
\begin{gathered}
P(X=x \mid Y=y), \quad \forall x, y \\
P(Y=y), \quad \forall y
\end{gathered}
$$

- We do not need to know $P(X=x), \forall x$


## Warm Up (Contd.)

- The probability that an image labeled by $y$ has feature vector $x$

$$
P(X=x \mid Y=y)=p_{X \mid Y}(x \mid y), \quad \forall x, y
$$

- The probability that an image is labeled by $y$

$$
P(Y=y)=p_{Y}(y), \quad \forall y
$$

- We compute the above parameters by learning from training data, but how?


## Warm Up (Contd.)

- Given a set of training data $\mathcal{D}=\left\{x^{(i)}, y^{(i)}\right\}_{i=1, \cdots, m}$
- The training data are sampled in an i.i.d. manner
- The probability of the $i$-th training data $\left(x^{(i)}, y^{(i)}\right)$

$$
\begin{aligned}
& P\left(X=x^{(i)}, Y=y^{(i)}\right) \\
= & P\left(X=x^{(i)} \mid Y=y^{(i)}\right) P\left(Y=y^{(i)}\right) \\
= & p_{X}\left(x^{(i)} \mid y^{(i)}\right) p_{Y}\left(y^{(i)}\right) \\
= & p_{X \mid Y}\left(x^{(i)} \mid y^{(i)}\right) p_{Y}\left(y^{(i)}\right)
\end{aligned}
$$

- The probability of $\mathcal{D}$

$$
P(\mathcal{D})=\prod_{i=1}^{m} p_{X \mid Y}\left(x^{(i)} \mid y^{(i)}\right) p_{Y}\left(y^{(i)}\right)
$$

## Warm Up (Contd.)

- Log-likelihood function

$$
\begin{aligned}
\ell(\theta) & =\log \prod_{i=1}^{m} p_{X, Y}\left(x^{(i)}, y^{(i)}\right) \\
& =\log \prod_{i=1}^{m} p_{X \mid Y}\left(x^{(i)} \mid y^{(i)}\right) p_{Y}\left(y^{(i)}\right) \\
& =\sum_{i=1}^{m}\left(\log p_{X \mid Y}\left(x^{(i)} \mid y^{(i)}\right)+\log p_{Y}\left(y^{(i)}\right)\right)
\end{aligned}
$$

where

$$
\theta=\left\{p_{X \mid Y}(x \mid y), p_{Y}(y)\right\}_{X, y}
$$

## Warm Up (Contd.)

- Suppose we have $n$ features

$$
X=\left[X_{1}, X_{2}, \cdots, X_{n}\right]^{T}
$$

- The features are independent with each other

$$
\begin{aligned}
P(X=x \mid Y=y) & =P\left(X_{1}=x_{1}, \cdots, X_{n}=x_{n} \mid Y=y\right) \\
& =\prod_{j=1}^{n} P\left(X_{j}=x_{j} \mid Y=y\right) \\
& =\prod_{j=1}^{n} p_{X_{j} \mid Y}\left(x_{j} \mid y\right)
\end{aligned}
$$

## Warm Up (Contd.)

- For each training data $\left(x^{(i)}, y^{(i)}\right)$

$$
\begin{aligned}
& P\left(X=x^{(i)} \mid Y=y^{(i)}\right) \\
= & P\left(X_{1}=x_{1}^{(i)}, \cdots, X_{n}=x_{n}^{(i)} \mid Y=y^{(i)}\right) \\
= & \prod_{j=1}^{n} P\left(X_{j}=x_{j}^{(i)} \mid Y=y^{(i)}\right) \\
= & \prod_{j=1}^{n} p_{X_{j} \mid Y}\left(x_{j}^{(i)} \mid y^{(i)}\right)
\end{aligned}
$$

## Gaussian Distribution

- Gaussian Distribution (Normal Distribution)

$$
p(x ; \mu, \sigma)=\frac{1}{\left(2 \pi \sigma^{2}\right)^{1 / 2}} \exp \left(-\frac{1}{2 \sigma^{2}}(x-\mu)^{2}\right)
$$

where $\mu$ is the mean and $\sigma^{2}$ is the variance

- Gaussian distributions are important in statistics and are often used in the natural and social science to represent real-valued random variables whose distribution are not known
- Central limit theorem: The averages of samples of observations of random variables independently drawn from independent distributions converge in distribution to the normal, that is, become normally distributed when the number of observations is sufficiently large
- Physical quantities that are expected to be the sum of many independent processes (such as measurement errors) often have distributions that are nearly normal.


## Multivariate Gaussian Distribution

- Multivariate normal distribution in $n$-dimensions $\mathcal{N}(\mu, \Sigma)$

$$
p(x ; \mu, \Sigma)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}(x-\mu)^{T} \Sigma^{-1}(x-\mu)\right)
$$

- Mean vector $\mu \in \mathbb{R}^{n}$
- Covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$
- Mahalanobis distance: $r^{2}=(x-\mu)^{T} \Sigma^{-1}(x-\mu)$
- $\Sigma$ is symmetric and positive semidefinite

$$
\Sigma=\Phi \wedge \Phi^{T}
$$

- $\Phi$ is an orthonormal matrix, whose columns are eigenvectors of $\Sigma$
- $\Lambda$ is a diagonal matrix with the diagonal elements being the eigenvalues


## Multivariate Gaussian Distribution: A 2D Example



From left to right: $\Sigma=I, \Sigma=0.6 /, \Sigma=2 l$




From left to right: $\Sigma=I, \Sigma=\left[\begin{array}{cc}1 & 0.5 \\ 0.5 & 1\end{array}\right], \Sigma=\left[\begin{array}{cc}1 & 0.8 \\ 0.8 & 1\end{array}\right]$

## Multivariate Gaussian Distribution: A 2D Example



## Gaussian Discriminant Analysis (Contd.)

- $Y \sim \operatorname{Bernoulli}(\psi)$
- $P(Y=1)=\psi$
- $P(Y=0)=1-\psi$
- Probability mass function

$$
p_{Y}(y)=\psi^{y}(1-\psi)^{1-y}, \quad \forall y=0,1
$$

## Gaussian Discriminant Analysis (Contd.)

- $X \mid Y=0 \sim \mathcal{N}\left(\mu_{0}, \Sigma\right)$
- Conditional probability density function of $X$ given $Y=0$

$$
p_{X \mid Y=0}(x)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{0}\right)^{T} \Sigma^{-1}\left(x-\mu_{0}\right)\right)
$$

- Or

$$
p_{X \mid Y}(x \mid 0)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{0}\right)^{T} \Sigma^{-1}\left(x-\mu_{0}\right)\right)
$$

## Gaussian Discriminant Analysis (Contd.)

- $X \mid Y=1 \sim \mathcal{N}\left(\mu_{1}, \Sigma\right)$
- Conditional probability density function of $X$ given $Y=1$

$$
p_{X \mid Y=1}(x)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{1}\right)^{T} \Sigma^{-1}\left(x-\mu_{1}\right)\right)
$$

- Or

$$
p_{X \mid Y}(x \mid 1)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{1}\right)^{T} \Sigma^{-1}\left(x-\mu_{1}\right)\right)
$$

## Gaussian Discriminant Analysis (Contd.)

- In summary, for $\forall y=0,1$

$$
\begin{aligned}
& p_{Y}(y)=\psi^{y}(1-\psi)^{1-y} \\
& p_{X \mid Y}(x \mid y)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{y}\right)^{T} \Sigma^{-1}\left(x-\mu_{y}\right)\right)
\end{aligned}
$$

## Gaussian Discriminant Analysis (Contd.)

- Given $m$ sample data, the log-likelihood is

$$
\begin{aligned}
& \ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right) \\
= & \log \prod_{i=1}^{m} p_{X, Y}\left(x^{(i)}, y^{(i)} ; \psi, \mu_{0}, \mu_{1}, \Sigma\right) \\
= & \log \prod_{i=1}^{m} p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{0}, \mu_{1}, \Sigma\right) p_{Y}\left(y^{(i)} ; \psi\right) \\
= & \sum_{i=1}^{m} \log p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{0}, \mu_{1}, \Sigma\right)+\sum_{i=1}^{m} \log p_{Y}\left(y^{(i)} ; \psi\right)
\end{aligned}
$$

## Gaussian Discriminant Analysis (Contd.)

- The log-likelihood function

$$
\ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=\sum_{i=1}^{m} \log p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{0}, \mu_{1}, \Sigma\right)+\sum_{i=1}^{m} \log p_{Y}\left(y^{(i)} ; \psi\right)
$$

- For each training data $\left(x^{(i)}, y^{(i)}\right)$
- If $y^{(i)}=0$

$$
p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{0}, \Sigma\right)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{0}\right)^{T} \Sigma^{-1}\left(x-\mu_{0}\right)\right)
$$

- If $y^{(i)}=1$

$$
p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{1}, \Sigma\right)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x-\mu_{1}\right)^{T} \Sigma^{-1}\left(x-\mu_{1}\right)\right)
$$

## Gaussian Discriminant Analysis (Contd.)

- The log-likelihood function

$$
\ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=\sum_{i=1}^{m} \log p_{X \mid Y}\left(x^{(i)} \mid y^{(i)} ; \mu_{0}, \mu_{1}, \Sigma\right)+\sum_{i=1}^{m} \log p_{Y}\left(y^{(i)} ; \psi\right)
$$

- For each training data $\left(x^{(i)}, y^{(i)}\right)$

$$
p_{Y}\left(y^{(i)} ; \psi\right)=\psi^{y^{(i)}}(1-\psi)^{1-y^{(i)}}
$$

## Gaussian Discriminant Analysis (Contd.)

- Maximizing $\ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)$ through

$$
\begin{aligned}
& \frac{\partial}{\partial \psi} \ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=0 \\
& \nabla_{\mu_{0}} \ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=0 \\
& \nabla_{\mu_{1}} \ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=0 \\
& \nabla_{\Sigma} \ell\left(\psi, \mu_{0}, \mu_{1}, \Sigma\right)=0
\end{aligned}
$$

## Gaussian Discriminant Analysis (Contd.)

- Solutions:

$$
\begin{aligned}
& \psi=\frac{1}{m} \sum_{i=1}^{m} \mathbf{1}\left\{y^{(i)}=1\right\} \\
& \mu_{0}=\sum_{i=1}^{m} \mathbf{1}\left\{y^{(i)}=0\right\} x^{(i)} / \sum_{i=1}^{m} \mathbf{1}\left\{y^{(i)}=0\right\} \\
& \mu_{1}=\sum_{i=1}^{m} \mathbf{1}\left\{y^{(i)}=1\right\} x^{(i)} / \sum_{i=1}^{m} \mathbf{1}\left\{y^{(i)}=1\right\} \\
& \Sigma=\frac{1}{m} \sum_{i=1}^{m}\left(x^{(i)}-\mu_{y^{(i)}}\right)\left(x^{(i)}-\mu_{y^{(i)}}\right)^{T}
\end{aligned}
$$

- Proof (see Problem Set 2)


## Gaussian Discriminant Analysis (Contd.)

- Given a test data sample $x$, we can calculate

$$
\begin{aligned}
p_{Y \mid X}(y=1 \mid x) & =\frac{p_{X \mid Y}(x \mid 1) p_{Y}(1)}{p_{X}(x)} \\
& =\frac{p_{X \mid Y}(x \mid 1) p_{Y}(1)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)+p_{X \mid Y}(x \mid 0) p_{Y}(0)} \\
& =\frac{1}{1+\frac{p_{X \mid Y}(x \mid 0) p_{Y}(0)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)}}
\end{aligned}
$$

## Gaussian Discriminant Analysis (Contd.)

$$
\begin{aligned}
& \frac{p_{X \mid Y}(x \mid 0) p_{Y}(0)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)} \\
= & \exp \left(-\frac{1}{2}\left(x-\mu_{0}\right)^{T} \Sigma^{-1}\left(x-\mu_{0}\right)+\frac{1}{2}\left(x-\mu_{1}\right)^{T} \Sigma^{-1}\left(x-\mu_{1}\right)\right) \cdot \frac{1-\psi}{\psi} \\
= & \exp \left(\left(\mu_{0}-\mu_{1}\right)^{T} \Sigma^{-1} x+\frac{1}{2}\left(\mu_{1}^{T} \Sigma^{-1} \mu_{1}-\mu_{0}^{T} \Sigma^{-1} \mu_{0}\right)\right) \cdot \exp \left(\log \left(\frac{1-\psi}{\psi}\right)\right) \\
= & \exp \left(\left(\mu_{0}-\mu_{1}\right)^{T} \Sigma^{-1} x+\frac{1}{2}\left(\mu_{1}^{T} \Sigma^{-1} \mu_{1}-\mu_{0}^{T} \Sigma^{-1} \mu_{0}\right)+\log \left(\frac{1-\psi}{\psi}\right)\right)
\end{aligned}
$$

## Gaussian Discriminant Analysis (Contd.)

- Assume

$$
x:=\left[\begin{array}{c}
x \\
1
\end{array}\right], \quad \theta=\left[\begin{array}{c}
\left(\mu_{0}-\mu_{1}\right)^{T} \Sigma^{-1} \\
\frac{1}{2}\left(\mu_{1}^{T} \Sigma^{-1} \mu_{1}-\mu_{0}^{T} \Sigma^{-1} \mu_{0}\right)+\log \left(\frac{1-\psi}{\psi}\right)
\end{array}\right]
$$

- We have

$$
\begin{aligned}
& \frac{p_{X \mid Y}(x \mid 0) p_{Y}(0)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)} \\
= & \exp \left(\left(\mu_{0}-\mu_{1}\right)^{T} \Sigma^{-1} x+\frac{\mu_{1}^{T} \Sigma^{-1} \mu_{1}-\mu_{0}^{T} \Sigma^{-1} \mu_{0}}{2}+\log \left(\frac{1-\psi}{\psi}\right)\right) \\
= & \exp \left(\theta^{T} x\right)
\end{aligned}
$$

- Then

$$
p_{Y \mid X}(1 \mid x)=\frac{1}{1+\frac{p_{X \mid Y}(x \mid 0) p_{Y}(y=0)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)}}=\frac{1}{1+\exp \left(\theta^{T} x\right)}
$$

## Gaussian Discriminant Analysis (Contd.)

- Similarly, we have

$$
\begin{aligned}
& p_{Y \mid X}(0 \mid x) \\
= & \frac{p_{X \mid Y}(x \mid 0) p_{Y}(0)}{p_{X}(x)} \\
= & \frac{p_{X \mid Y}(x \mid 0) p_{Y}(0)}{p_{X \mid Y}(x \mid 1) p_{Y}(1)+p_{X \mid Y}(x \mid 0) p_{Y}(y=0)} \\
= & \frac{1}{1+\frac{p_{X \mid Y}(x \mid 1) p_{Y}(1)}{p_{X \mid Y}(x \mid 0) p_{Y}(y=0)}} \\
= & \frac{1}{1+\exp \left(\left(\mu_{1}-\mu_{0}\right)^{T} \Sigma^{-1} x+\frac{\mu_{0}^{T} \Sigma^{-1} \mu_{0}-\mu_{1}^{T} \Sigma^{-1} \mu_{1}}{2}+\log \left(\frac{\psi}{1-\psi}\right)\right)}
\end{aligned}
$$

## GDA and Logistic Regression

- GDA model can be reformulated as logistic regression
- Which one is better?
- GDA makes stronger modeling assumptions, and is more data efficient (i.e., requires less training data to learn "well") when the modeling assumptions are correct or at least approximately correct
- Logistic regression makes weaker assumptions, and is significantly more robust deviations from modeling assumptions
- When the data is indeed non-Gaussian, then in the limit of large datasets, logistic regression will almost always do better than GDA
- In practice, logistic regression is used more often than GDA


## Gaussian Discriminant Analysis (Contd.)



## Lagrange Multiplier

## Theorem (Lagrange Multiplier Theorem)

Let $f: \mathbb{R}^{n} \rightarrow R$ be the objective function, $g_{j}: \mathbb{R}^{n} \rightarrow R($ with $j=1, \cdots, m)$ be the $m$ constraints functions, all of which have continuous fist derivatives. Let $x^{*}$ be an optimal solution to the following optimization problem

$$
\begin{array}{cl}
\max & f(x) \\
\text { s.t. } & g_{i}(x)=0, i=1,2, \cdots, m
\end{array}
$$

such that $\operatorname{Rank}\left(D g\left(x^{*}\right)\right)=m<n$ where $\operatorname{Rank}\left(D g\left(x^{*}\right)\right)$ denotes the matrix of partial derivatives $\left[\frac{\partial g_{j}}{\partial x_{i}}\right]$. There exist unique Lagrange multipliers $\lambda \in \mathbb{R}^{m}$ such that

$$
\nabla f\left(x^{*}\right)=\sum_{j=1}^{m} \lambda_{j} \nabla g_{j}\left(x^{*}\right)
$$

## Lagrange Multiplier

- Maximize $f(x, y)$ subject to $g(x, y)=0$
- $f(x, y)$ is maximized at point $\left(x_{0}, y_{0}\right)$ where they have common tangent line such that the gradient vectors are parallel

$$
\begin{aligned}
& \nabla f\left(x_{0}, y_{0}\right)=\lambda \nabla g\left(x_{0}, y_{0}\right) \\
& \hline 0 \\
& f(x, y)=0 \\
& f(x, y)=11 \\
& f(x, y)=10 \\
& f(x, y)=9
\end{aligned}
$$

- How about higher dimension?


## Lagrange Multiplier (Contd.)

- Maximize $f(x, y, z)$ subject to $g(x, y, z)=0$
- $r(t)=(x(t), y(t), z(t))$ be an arbitrary parameterized curve which lies on the constraint surface and has $(x(0), y(0), z(0))=q$
- Suppose $h(t)=f(x(t), y(t), z(t))$ such that $h(t)$ has a maximum at $t=0$
- By the chain rule

$$
h^{\prime}(t)=\left.\nabla f\right|_{r(t)} \cdot r^{\prime}(t)
$$

- Since $t=0$ is a local maximum, we have

$$
h^{\prime}(0)=\left.\nabla f\right|_{q} \cdot r^{\prime}(0)=0
$$

- $\left.\nabla f\right|_{q}$ is perpendicular to any curve on the constraint surface through $q$, which implies $\left.\nabla f\right|_{q}$ is perpendicular to the surface
- Since $\left.\nabla g\right|_{q}$ is also perpendicular to the surface, we have proved $\nabla f_{q}$ is parallel to $\left.\nabla g\right|_{q}$


## Lagrange Multiplier (Contd.)

- How about multiple constraints?

$$
\begin{array}{cl}
\max & f(x) \\
\text { s.t. } & g_{i}(x)=0, i=1,2, \cdots, m
\end{array}
$$

where $x \in \mathbb{R}^{n}, f: \mathbb{R}^{n} \rightarrow R$, and $g_{i}: \mathbb{R}^{n} \rightarrow R$ for $\forall i=1, \cdots, m$

- $\left.\nabla f\right|_{q}$ is "perpendicular" to all "constraint surface"
- $\left.\nabla f\right|_{q}$ is in the plane determined by $\left.\nabla g_{i}\right|_{q}(i=1, \cdots, m)$


## Spam Email Classifier

- Given an email with fixed length, is it a spam?
- Training a (binary) classifier according to a data set $\left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1, \cdots, m}$
- Each data sample is a $n$-dimensional vector

$$
x^{(i)}=\left(x_{1}^{(i)}, x_{2}^{(i)}, \cdots, x_{n}^{(i)}\right)
$$

where $x_{j}^{(i)}$ indicates if the $j$-th word in the dictionary occurring in the email

- For example,

$$
x=\left[\begin{array}{c}
1 \\
0 \\
0 \\
\text { aardvark } \\
\text { aardwolf } \\
\vdots \\
1 \\
\vdots \\
\vdots \\
0
\end{array}\right] \begin{gathered}
\text { buy } \\
\text { zygmurgy }
\end{gathered}
$$

## Spam Email Classifier (Contd.)

- Given an email with fixed length, is it a spam?
- Training a (binary) classifier according to a data set $\left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1, \ldots, m}$
- Each data sample is a $n$-dimensional vector

$$
x^{(i)}=\left(x_{1}^{(i)}, x_{2}^{(i)}, \cdots, x_{n}^{(i)}\right)
$$

where $x_{j}^{(i)} \in\{0,1\}$ indicates if the $j$-th word in the dictionary occurring in the email

- $y^{(i)} \in\{0,1\}$ indicates if the $i$-th email is a spam


## Naive Bayes

- Training data $\left(x^{(i)}, y^{(i)}\right)_{i=1, \cdots, m}$
- $x^{(i)}$ is a $n$-dimensional vector
- Each feature $x_{j}^{(i)} \in\{0,1\}(j=1, \cdots, n)$
- $y^{(i)} \in\{0,1\}$
- The features and labels can be represented by random variables $\left\{X_{j}\right\}_{j=1, \cdots}$, and $Y$, respectively


## Naive Bayes (Contd.)

- For $\forall j \neq j^{\prime}$, Naive Bayes assumes $X_{j}$ and $X_{j^{\prime}}$ are conditionally independent given $Y$

$$
\begin{aligned}
& P\left(X_{1}=x_{1}, X_{2}=x_{2}, \cdots, X_{n}=x_{n} \mid Y=y\right) \\
= & \prod_{j=1}^{n} P\left(X_{j}=x_{j} \mid X_{1}=x_{1}, X_{2}=x_{2}, \cdots, X_{j-1}=x_{j-1}, Y=y\right) \\
= & \prod_{j=1}^{n} P\left(X_{j}=x_{j} \mid Y=y\right)
\end{aligned}
$$

## Naive Bayes (Contd.)

- The key assumption in NB model

$$
\begin{aligned}
& P\left(Y=y, X_{1}=x_{1}, \cdots, X_{n}=x_{n}\right) \\
= & P\left(X_{1}=x_{1}, \cdots, X_{n}=x_{n} \mid Y=y\right) P(Y=y) \\
= & P(Y=y) \prod_{j=1}^{n} P\left(X_{j}=x_{j} \mid Y=y\right) \\
= & p_{Y}(y) \prod_{j=1}^{n} p_{X_{j} \mid Y}\left(x_{j} \mid y\right)
\end{aligned}
$$

- Dropping the subscripts will not induce any ambiguity

$$
P\left(Y=y, X_{1}=x_{1}, \cdots, X_{n}=x_{n}\right)=p(y) \prod_{j=1}^{n} p_{j}\left(x_{j} \mid y\right)
$$

## Naive Bayes (Contd.)

- Two sets of parameters (denoted by $\Omega$ )
- Probability mass function of $Y$

$$
p(y)=P(Y=y)
$$

where $\forall y \in\{0,1\}$

- Conditional probability mass function of $X_{j}(j \in\{1,2, \cdots, n\})$ given $Y=y(y \in\{0,1\})$

$$
p_{j}(x \mid y)=P\left(X_{j}=x \mid Y=y\right)
$$

where $\forall x_{j} \in\{0,1\}$

## Maximum-Likelihood Estimates for Naive Bayes

- Log-likelihood function is

$$
\begin{aligned}
\ell(\Omega) & =\log \prod_{i=1}^{m} p\left(x^{(i)}, y^{(i)}\right) \\
& =\sum_{i=1}^{m} \log p\left(x^{(i)}, y^{(i)}\right) \\
& =\sum_{i=1}^{m} \log \left(p\left(y^{(i)}\right) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y^{(i)}\right)\right) \\
& =\sum_{i=1}^{m} \log p\left(y^{(i)}\right)+\sum_{i=1}^{m} \sum_{j=1}^{n} \log p_{j}\left(x_{j}^{(i)} \mid y^{(i)}\right)
\end{aligned}
$$

## MLE for Naive Bayes (Contd.)

$$
\begin{array}{ll}
\max & \sum_{i=1}^{m} \log p\left(y^{(i)}\right)+\sum_{i=1}^{m} \sum_{j=1}^{n} \log p_{j}\left(x_{j}^{(i)} \mid y^{(i)}\right) \\
\text { s.t. } & \sum_{y \in\{0,1\}} p(y)=1 \\
& \sum_{x \in\{0,1\}} p_{j}(x \mid y)=1, \forall y, j \\
& p(y) \geq 0, \forall y \\
& p_{j}(x \mid y) \geq 0, \forall j, x, y
\end{array}
$$

## MLE for Naive Bayes (Contd.)

- Theorem 1

The maximum-likelihood estimates for Naive Bayes model are as follows

$$
p(y)=\frac{\operatorname{count}(y)}{m}=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)}{m}, \forall y
$$

and

$$
p_{j}(x \mid y)=\frac{\operatorname{count}_{j}(x \mid y)}{\operatorname{count}(y)}=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y \wedge x_{j}^{(i)}=x\right)}{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)}, \forall x, y, j
$$

## MLE for Naive Bayes (Contd.)

- Notation:
- The number of training data whose label is $y$

$$
\operatorname{count}(y)=\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right), \forall y=0,1
$$

- The number of training data with the $j$-th feature being $x$ and the label being $y$

$$
\operatorname{count}_{j}(x \mid y)=\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y \wedge x_{j}^{(i)}=x\right), \forall y=0,1, \forall x=0,1
$$

## MLE for Naive Bayes (Contd.)

- What if $x \in\{1,2, \cdots, u\}$ and $y \in\{1,2, \cdots, k\}$ ?
- Can we get the same results? Check it yourself!


## Classification by Naive Bayes

- Given a test sample $\tilde{x}=\left[\tilde{x}_{1}, \tilde{x}_{2}, \cdots, \tilde{x}_{n}\right]^{\top}$, we have

$$
\begin{aligned}
& P\left(Y=y \mid X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n}\right) \\
= & \frac{P\left(X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n} \mid Y=y\right) P(Y=y)}{P\left(X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n}\right)} \\
= & \frac{P(Y=y) \prod_{j=1}^{n} P\left(X_{j}=\tilde{x}_{j} \mid Y=y\right)}{P\left(X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n}\right)} \\
= & \frac{p(y) \prod_{j=1}^{n} p_{j}\left(\tilde{x}_{j} \mid y\right)}{p\left(\tilde{x}_{1}, \cdots, \tilde{x}_{n}\right)}
\end{aligned}
$$

- Therefore, the output of the Naive Bayes model is

$$
\arg \max _{y \in\{0,1\}}\left(p(y) \prod_{j=1}^{n} p_{j}\left(\tilde{x}_{j} \mid y\right)\right)
$$

## Classification by Naive Bayes (Contd.)

- Example: $y=0,1$

$$
\begin{aligned}
& P\left(Y=0 \mid X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n}\right)=\frac{p_{Y}(0) \prod_{j=1}^{n} p_{X_{j} \mid Y}\left(\tilde{x}_{j} \mid 0\right)}{p_{X}\left(\tilde{x}_{1}, \cdots, \tilde{x}_{n}\right)} \\
& P\left(Y=1 \mid X_{1}=\tilde{x}_{1}, \cdots, X_{n}=\tilde{x}_{n}\right)=\frac{p_{Y}(1) \prod_{j=1}^{n} p_{X_{j} \mid Y}\left(\tilde{x}_{j} \mid 1\right)}{p_{X}\left(\tilde{x}_{1}, \cdots, \tilde{x}_{n}\right)}
\end{aligned}
$$

## Laplace Smoothing

- There may exist some feature, e.g., $X_{j^{*}}$, such that $X_{j^{*}}=1$ for some $x^{*}$ may never happen in the training data

$$
p_{j^{*}}\left(x_{j^{*}}=1 \mid y\right)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y \wedge x_{\dot{j}^{*}}^{(i)}=1\right)}{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)}=0, \forall y=0,1
$$

- As a result, given a test data $x$ with $x_{j^{*}}=1$

$$
p(y \mid x)=\frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j} \mid y\right)}{\sum_{y} \prod_{j=1}^{n} p_{j}\left(x_{j} \mid y\right) p(y)}=\frac{0}{0}, \quad \forall y=0,1
$$

## Laplace Smoothing (Contd.)

- This is unreasonable!!!
- How can we resolve this problem?
- Laplace smoothing:

$$
\begin{aligned}
& p(y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)+1}{m+k} \\
& p_{j}(x \mid y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y \wedge x_{j}^{(i)}=x\right)+1}{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)+v_{j}}
\end{aligned}
$$

where $k$ is number of the possible values of $y$ ( $k=2$ in our case), and $v_{j}$ is the number of the possible values of the $j$-th feature ( $v_{j}=2$ for $\forall j=1, \cdots, n$ in our case)

## Naive Bayes for Multinomial Distribution

- Let's go back to the spam classification problem
- Each training sample (as well as the test data) has different length

$$
x^{(i)}=\left[x_{1}^{(i)}, x_{2}^{(i)}, \cdots, x_{n_{i}}^{(i)}\right]^{\mathrm{T}}
$$

- The $j$-th feature of $x^{(i)}$ takes a finite set of values

$$
x_{j}^{(i)} \in\{1,2, \cdots, v\}, \text { for } \forall j=1, \cdots, n_{i}
$$

- For example, $x_{j}^{(i)}$ indicates the $j$-th word in the email
- Specifically, $x_{j}^{(i)}=3$ implies the $j$-th word in the email is the 3 rd on in the dictionary


## Naive Bayes for Multinomial Distribution (Contd.)

- Assumptions:
- Each training sample involves a different number of features

$$
x^{(i)}=\left[x_{1}^{(i)}, x_{2}^{(i)}, \cdots, x_{n_{i}}^{(i)}\right]^{\mathrm{T}}
$$

- The $j$-th feature of $x^{(i)}$ takes a finite set of values

$$
x_{j}^{(i)} \in\{1,2, \cdots, v\}, \text { for } \forall j=1, \cdots, n_{i}
$$

- For each training data, the features are i.i.d.

$$
P\left(X_{j}=t \mid Y=y\right)=p(t \mid y), \text { for } \forall j=1, \cdots, n_{i}
$$

- $p(t \mid y) \geq 0$ is the conditional probability mass function of $X_{j} \mid Y=y$
- $\sum_{t=1}^{v} p(t \mid y)=1$


## Naive Bayes for Multinomial Distribution (Contd.)

- Assumptions:
- Each training sample involves a different number of features

$$
x^{(i)}=\left[x_{1}^{(i)}, x_{2}^{(i)}, \cdots, x_{n_{i}}^{(i)}\right]^{\mathrm{T}}
$$

- The $j$-th feature of $x^{(i)}$ takes a finite set of values, $x_{j}^{(i)} \in\{1,2, \cdots, v\}$
- For each training data $\left(x^{(i)}, y^{(i)}\right)$ where $x^{(i)}$ is a $n_{i}$-dimensional vector

$$
\begin{aligned}
& P\left(Y=y^{(i)}\right)=p\left(y^{(i)}\right) \\
& P\left(X=x^{(i)} \mid Y=y^{(i)}\right)=\prod_{j=1}^{n_{i}} p\left(x_{j}^{(i)} \mid y^{(i)}\right)
\end{aligned}
$$

## Naive Bayes for Multinomial Distribution (Contd.)

- Log-likelihood function $\left(\Omega=\{p(y), p(t \mid y)\}_{y \in\{0,1\}, t \in\{1, \cdots, v\}}\right)$

$$
\begin{aligned}
\ell(\Omega) & =\log \prod_{i=1}^{m} p\left(x^{(i)}, y^{(i)}\right) \\
& =\sum_{i=1}^{m} \log p\left(x^{(i)} \mid y^{(i)}\right) p\left(y^{(i)}\right) \\
& =\sum_{i=1}^{m} \log p\left(y^{(i)}\right) \prod_{j=1}^{n_{i}} p\left(x_{j}^{(i)} \mid y^{(i)}\right) \\
& =\sum_{i=1}^{m} \sum_{j=1}^{n_{i}} \log p\left(x_{j}^{(i)} \mid y^{(i)}\right)+\sum_{i=1}^{m} \log p\left(y^{(i)}\right)
\end{aligned}
$$

## Naive Bayes for Multinomial Distribution (Contd.)

- Problem formulation

$$
\begin{array}{ll}
\max & \ell(\Omega)=\sum_{i=1}^{m} \sum_{j=1}^{n_{i}} \log p\left(x_{j}^{(i)} \mid y^{(i)}\right)+\sum_{i=1}^{m} \log p\left(y^{(i)}\right) \\
\text { s.t. } & \sum_{y \in\{0,1\}} p(y)=1 \\
& \sum_{t=1}^{v} p(t \mid y)=1, \forall y=0,1 \\
& p(y) \geq 0, \forall y=0,1 \\
& p(t \mid y) \geq 0, \forall t=1, \cdots, v, \forall y=0,1
\end{array}
$$

## Naive Bayes for Multinomial Distribution (Contd.)

- Solution

$$
\begin{aligned}
& p(t \mid y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right) \operatorname{count}^{(i)}(t)}{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right) \sum_{t=1}^{v} \operatorname{count}^{(i)}(t)} \\
& p(y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)}{m} \\
& \text { where } \operatorname{count}^{(i)}(t)=\sum_{j=1}^{n_{i}} \mathbf{1}\left(x_{j}^{(i)}=t\right)
\end{aligned}
$$

- Check them by yourselves!
- What if $y=1,2, \cdots, k$ ?


## Naive Bayes for Multinomial Distribution (Contd.)

- Laplace smoothing

$$
\begin{gathered}
\psi(t \mid y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right) \operatorname{count}^{(i)}(t)+1}{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right) \sum_{t=1}^{v} \operatorname{count}^{(i)}(t)+v} \\
\psi(y)=\frac{\sum_{i=1}^{m} \mathbf{1}\left(y^{(i)}=y\right)+1}{m+k}
\end{gathered}
$$

## Convex Functions

- A set $C$ is convex if the line segment between any two points in $C$ lies in $C$, i.e., for $\forall x_{1}, x_{2} \in C$ and $\forall \theta$ with $0 \leq \theta \leq 1$, we have

$$
\theta x_{1}+(1-\theta) x_{2} \in C
$$

- A function $f: \mathbb{R}^{n} \rightarrow R$ is convex, if $\operatorname{dom} f$ is a convex set and if for all $x, y \in \operatorname{dom} f$ and $\lambda$ with $0 \leq \lambda \leq 1$, we have

$$
f(\lambda x+(1-\lambda) y) \leq \lambda f(x)+(1-\lambda) f(y)
$$



## Convex Functions (Contd.)

- First-order conditions: Suppose $f$ is differentiable (i.e., its gradient $\nabla f$ exists at each point in $\operatorname{dom} f$, which is open). Then, $f$ is convex if and only if $\operatorname{dom} f$ is convex and

$$
f(y) \geq f(x)+\nabla f(x)^{T}(y-x)
$$

holds for $\forall x, y \in \operatorname{dom} f$


## Convex Functions (Contd.)

- Second-order conditions: Assume $f$ is twice differentiable (i.t., its Hessian matrix or second derivative $\nabla^{2} f$ exists at each point in $\operatorname{dom} f$, which is open), then $f$ is convex if and only if dom $f$ is convex and its Hessian is positive semidefinite: for $\forall x \in \operatorname{dom} f$,

$$
\nabla^{2} f \succeq 0
$$

## Jensen's Inequality

- Let $f$ be a convex function, then

$$
f\left(\lambda x_{1}+(1-\lambda) x_{2}\right) \leq \lambda f\left(x_{1}\right)+(1-\lambda) f\left(x_{2}\right)
$$

where $\lambda \in[0,1]$

- Jensen's Inequality
- Let $f(x)$ be a convex function defined on an interval $\mathcal{I}$. If $x_{1}, x_{2}, \cdots, x_{N} \in$ $\mathcal{I}$ and $\lambda_{1}, \lambda_{2}, \cdots, \lambda_{N} \geq 0$ with $\sum_{i=1}^{N} \lambda_{i}=1$

$$
f\left(\sum_{i=1}^{N} \lambda_{i} x_{i}\right) \leq \sum_{i=1}^{N} \lambda_{i} f\left(x_{i}\right)
$$

## The Proof of Jensen's Inequality

- When $N=1$, the result is trivial
- When $N=2$,

$$
f\left(\lambda_{1} x_{1}+\lambda_{2} x_{2}\right) \leq \lambda_{1} f\left(x_{1}\right)+\lambda_{2} f\left(x_{2}\right)
$$

due to convexity of $f(x)$

- When $N \geq 3$, the proof is by induction
- We assume that, the Jensen's inequality holds when $N=k-1$.

$$
f\left(\sum_{i=1}^{k-1} \lambda_{i} x_{i}\right) \leq \sum_{i=1}^{k-1} \lambda_{i} f\left(x_{i}\right)
$$

- We then prove that, the Jensen's inequality still holds for $N=k$


## The Proof of Jensen's Inequality (Contd.)

- When $N=k$,

$$
\begin{aligned}
f\left(\sum_{i=1}^{k} \lambda_{i} x_{i}\right) & =f\left(\sum_{i=1}^{k-1} \lambda_{i} x_{i}+\lambda_{k} x_{k}\right) \\
& =f\left(\left(1-\lambda_{k}\right) \sum_{i=1}^{k-1} \frac{\lambda_{i}}{1-\lambda_{k}} x_{i}+\lambda_{k} x_{k}\right) \\
& \leq\left(1-\lambda_{k}\right) f\left(\sum_{i=1}^{k-1} \frac{\lambda_{i}}{1-\lambda_{k}} x_{i}\right)+\lambda_{k} f\left(x_{k}\right) \\
& \leq\left(1-\lambda_{k}\right) \sum_{i=1}^{k-1} \frac{\lambda_{i}}{1-\lambda_{k}} f\left(x_{i}\right)+\lambda_{k} f\left(x_{k}\right) \\
& =\sum_{i=1}^{k-1} \lambda_{i} f\left(x_{i}\right)+\lambda_{k} f\left(x_{k}\right)=\sum_{i=1}^{k} \lambda_{i} f\left(x_{i}\right)
\end{aligned}
$$

## The Probabilistic Form of Jensen's Inequality

- The inequality can be extended to infinite sums, integrals, and expected values
- If $p(x) \geq 0$ on $\mathcal{S} \subseteq \operatorname{dom} f$ and $\int_{\mathcal{S}} p(x) d x=1$, we have

$$
f\left(\int_{\mathcal{S}} p(x) x d x\right)=\int_{\mathcal{S}} p(x) f(x) d x
$$

- Assuming $X$ is a random variable and $P$ is a probability distribution on sample space $\mathcal{S}$, we have

$$
f[E(X)] \leq E[f(X)]
$$

- The equality holds if $X$ is a constant


## Jensen's inequality for Concave Function

- Assume $f$ be a concave function

$$
f\left(\sum_{i=1}^{N} \lambda_{i} x_{i}\right) \geq \sum_{i=1}^{N} \lambda_{i} f\left(x_{i}\right)
$$

- The probabilistic form

$$
f(E[X]) \geq E[f(X)]
$$

- Example: $f(x)=\log x$
- $\log \left(\sum_{i=1}^{N} \lambda_{i} x_{i}\right) \geq \sum_{i=1}^{N} \lambda_{i} \log \left(x_{i}\right)$
- $\log (E[X]) \geq E[\log (X)]$


## The Expectation-Maximization (EM) Algorithm

- A training set $\left\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\right\}$ (without labels)
- The log-likelihood function

$$
\begin{aligned}
\ell(\theta) & =\log \prod_{i=1}^{m} p\left(x^{(i)} ; \theta\right) \\
& =\sum_{i=1}^{m} \log \sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right)
\end{aligned}
$$

- $\theta$ denotes the full set of unknown parameters in the model - $z^{(i)} \in \Omega$ is so-called "latent variable"


## The EM Algorithm (Contd.)

- Our goal is to maximize the log-likelihood function

$$
\ell(\theta)=\sum_{i=1}^{m} \log \sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right)
$$

- The basic idea of EM algorithm
- Repeatedly construct a lower-bound on $\ell$ (E-step)
- Then optimize that lower-bound (M-step)


## The EM Algorithm (Contd.)

- $Q_{i}$ : The probability distribution of the (latent) variable of the $i$-th training sample

$$
\sum_{z \in \Omega} Q_{i}(z)=1, \quad Q_{i}(z) \geq 0
$$

- We have

$$
\begin{aligned}
\ell(\theta) & =\sum_{i=1}^{m} \log \sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right) \\
& =\sum_{i=1}^{m} \log \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}
\end{aligned}
$$

## The EM Algorithm (Contd.)

- Re-visit the log-likelihood function

$$
\begin{aligned}
\ell(\theta) & =\sum_{i=1}^{m} \log \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)} \\
& =\sum_{i=1}^{m} \log E\left[\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}\right]
\end{aligned}
$$

## The EM Algorithm (Contd.)

- Since $\log (\cdot)$ is a concave function, according to Jensen's inequality, we have

$$
\log \left(E\left[\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}\right]\right) \geq E\left[\log \left(\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}\right)\right]
$$

- Then, the log-likelihood function

$$
\begin{aligned}
\ell(\theta) & =\sum_{i=1}^{m} \log \left(E\left[\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}\right]\right) \\
& \geq \sum_{i=1}^{m} E\left[\log \left(\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}\right)\right] \\
& =\sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}
\end{aligned}
$$

## The EM Algorithm (Contd.)

- For any set of distributions $Q_{i}, \ell(\theta)$ has a lower bound

$$
\ell(\theta) \geq \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}
$$

- Tighten the lower bound (i.e., let the equality hold)
- The equality in the Jensen's inequality holds if

$$
\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}=c
$$

where $c$ is a constant

## The EM Algorithm (Contd.)

- Tighten the lower bound (i.e., let the equality hold)
- The equality in the Jensen's inequality holds if

$$
\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}=c
$$

where $c$ is a constant

- Since

$$
\sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right)=1
$$

we have

$$
\sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right)=c \sum_{z^{(i)} \in \Omega} Q_{i}(z)=c
$$

- Tighten the lower bound (i.e., let the equality hold)
- We have

$$
\left\{\begin{array}{l}
p\left(x^{(i)}, z^{(i)} ; \theta\right) / Q_{i}\left(z^{(i)}\right)=c \\
\sum_{z^{(i)} \in \Omega} Q_{i}(z)=1 \\
\sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right)=c
\end{array}\right.
$$

- Therefore,

$$
\begin{aligned}
Q_{i}\left(z^{(i)}\right) & =\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{c} \\
& =\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{\sum_{z^{(i)} \in \Omega} p\left(x^{(i)}, z^{(i)} ; \theta\right)} \\
& =\frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{p\left(x^{(i)} ; \theta\right)} \\
& =p\left(z^{(i)} \mid x^{(i)} ; \theta\right)
\end{aligned}
$$

## The EM Algorithm (Contd.)

- Repeat the following step until convergence
- (E-step) For each $i$, set

$$
Q_{i}\left(z^{(i)}\right):=p\left(z^{(i)} \mid x^{(i)} ; \theta\right)
$$

- (M-step) set

$$
\theta:=\arg \max _{\theta} \sum_{i} \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}
$$

## Convergence

- For the $t$-th iteration, the equality in the Jensen's inequality holds with respect to $\theta^{[t]}$

$$
\ell\left(\theta^{[t]}\right)=\sum_{i=1}^{m} \sum_{z^{(i)}} Q_{i}^{[t]}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta^{[t]}\right)}{Q_{i}^{[t]}\left(z^{(i)}\right)}
$$

where $Q_{i}^{[t]}\left(z^{(i)}\right)=p\left(z^{(i)} \mid x^{(i)} ; \theta^{[t]}\right)$

- $\theta^{[t+1]}$ is then obtained by maximizing the right hand side of the above equation


## Convergence (Contd.)

- Since $\ell(\theta)$ has a lower bound

$$
\ell(\theta) \geq \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}\left(z^{(i)}\right)}
$$

for $\forall Q_{i}$ and $\theta$, we have

$$
\ell\left(\theta^{[t+1]}\right) \geq \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}^{[t]}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta^{[t+1]}\right)}{Q_{i}^{[t]}\left(z^{(i)}\right)}
$$

## Convergence (Contd.)

- Since

$$
\theta^{[t+1]}=\arg \max _{\theta} \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}^{[t]}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta\right)}{Q_{i}^{[t]}\left(z^{(i)}\right)}
$$

we have

$$
\begin{aligned}
\ell\left(\theta^{[t+1]}\right) & \geq \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}^{[t]}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta^{[t+1]}\right)}{Q_{i}^{[t]}\left(z^{(i)}\right)} \\
& \geq \sum_{i=1}^{m} \sum_{z^{(i)} \in \Omega} Q_{i}^{[t]}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \theta^{[t]}\right)}{Q_{i}^{[t]}\left(z^{(i)}\right)} \\
& =\ell\left(\theta^{[t]}\right)
\end{aligned}
$$

## Reviewing Mixtures of Gaussians

- A training set $\left\{x^{(1)}, \cdots, x^{(m)}\right\}$
- Mixture of Gaussians model

$$
p_{X, Z}(x, z)=p_{X \mid Z}(x \mid z) p_{Z}(z)
$$

- $Z \in\{1, \cdots, k\} \sim \operatorname{Multinomial}\left(\phi_{1}, \phi_{2}, \cdots, \phi_{k}\right)$
- $\phi_{j}=P(Z=j)$ such that $\phi_{j} \geq 0$ and $\sum_{j=1}^{k} \phi_{j}=1$
- $X \mid Z=j \sim \mathcal{N}\left(\mu_{j}, \Sigma_{j}\right)($ for $j=1,2, \cdots, k)$
- Z's are so-called latent random variables, since they are hidden/unobserved


## Reviewing Mixtures of Gaussians (Contd.)

- The log-likelihood function

$$
\begin{aligned}
\ell(\phi, \mu, \Sigma) & =\sum_{i=1}^{m} \log p\left(x^{(i)} ; \phi, \mu, \Sigma\right) \\
& =\sum_{i=1}^{m} \log \sum_{z^{(i)}=1}^{k} p\left(x^{(i)} \mid z^{(i)} ; \mu, \Sigma\right) p\left(z^{(i)} ; \phi\right)
\end{aligned}
$$

## Applying EM Algorithm to Mixtures of Gaussians

- Repeat the following steps until convergence
- (E-step) For each $i, j$, set

$$
\omega_{j}^{(i)}=\frac{p\left(x^{(i)} \mid z^{(i)}=j ; \mu, \Sigma\right) p\left(z^{(i)}=j ; \phi\right)}{\sum_{l=1}^{k} p\left(x^{(i)} \mid z^{(i)}=l ; \mu, \Sigma\right) p\left(z^{(i)}=I ; \phi\right)}
$$

- (M-step) Update the parameters

$$
\begin{aligned}
& \phi_{j}=\frac{1}{m} \sum_{i=1}^{m} \omega_{j}^{(i)} \\
& \mu_{j}=\frac{\sum_{i=1}^{m} \omega_{j}^{(i)} x^{(i)}}{\sum_{i=1}^{m} \omega_{j}^{(i)}} \\
& \Sigma_{j}=\frac{\sum_{i=1}^{m} \omega_{j}^{(i)}\left(x^{(i)}-\mu_{j}\right)\left(x^{(i)}-\mu_{j}\right)^{T}}{\sum_{i=1}^{m} \omega_{j}^{(i)}}
\end{aligned}
$$

## Applying EM Algorithm to MG (Contd.)

- (E-step) For each $i, j$, set

$$
\begin{aligned}
\omega_{j}^{(i)} & =Q_{i}\left(z^{(i)}=j\right) \\
& =p\left(z^{(i)}=j \mid x^{(i)} ; \phi, \mu, \Sigma\right) \\
& =\frac{p\left(x^{(i)} \mid z^{(i)}=j ; \mu, \Sigma\right) p\left(z^{(i)}=j ; \phi\right)}{\sum_{l=1}^{k} p\left(x^{(i)} \mid z^{(i)}=l ; \mu, \Sigma\right) p\left(z^{(i)}=l ; \phi\right)}
\end{aligned}
$$

where
$p\left(x^{(i)} \mid z^{(i)}=j ; \mu_{j}, \Sigma_{j}\right)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)\right)$
$p\left(z^{(i)}=j ; \phi\right)=\phi_{j}$

## Applying EM Algorithm to MG (Contd.)

- (M-step) Maximizing

$$
\begin{aligned}
& \sum_{i=1}^{m} \sum_{z^{(i)}} Q_{i}\left(z^{(i)}\right) \log \frac{p\left(x^{(i)}, z^{(i)} ; \phi, \mu, \Sigma\right)}{Q_{i}\left(z^{(i)}\right)} \\
= & \sum_{i=1}^{m} \sum_{j=1}^{k} Q_{i}\left(z^{(i)}=j\right) \log \frac{p\left(x^{(i)} \mid z^{(i)}=j ; \mu, \Sigma\right) p\left(z^{(i)}=j ; \phi\right)}{Q_{i}\left(z^{(i)}=j\right)} \\
= & \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \frac{\frac{1}{(2 \pi)^{n / 2}\left|\Sigma_{j}\right|^{1 / 2}} \exp \left(-\frac{1}{2}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)\right) \phi_{j}}{\omega_{j}^{(i)}} \\
= & -\sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}\left[\log \left((2 \pi)^{\frac{n}{2}}\left|\Sigma_{j}\right|^{\frac{1}{2}}\right)+\frac{1}{2}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)\right] \\
& +\sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \phi_{j}-\sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \omega_{j}^{(i)}
\end{aligned}
$$

## Applying EM Algorithm to MG: Calculating $\mu$

Since

$$
\begin{aligned}
& \nabla \mu_{l} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \frac{\frac{1}{(2 \pi)^{n / 2}\left|\Sigma_{j}\right|^{1 / 2}}}{} \exp \left(-\frac{1}{2}\left(x^{(j)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(j)}-\mu_{j}\right)\right) \phi_{j} \\
& \omega_{j}^{(i)} \\
&= \nabla \mu_{l} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \frac{1}{2}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right) \\
&= \frac{1}{2} \sum_{i=1}^{m} \omega_{l}^{(i)} \nabla \mu_{l}\left(2 \mu_{l}^{T} \Sigma_{l}^{-1} x^{(i)}-\mu_{l}^{T} \Sigma_{l}^{-1} \mu_{l}\right) \\
&= \sum_{i=1}^{m} \omega_{l}^{(i)}\left(\Sigma_{l}^{-1} x^{(i)}-\Sigma_{l}^{-1} \mu_{l}\right)=0
\end{aligned}
$$

we have

$$
\mu_{I}=\frac{\sum_{i=1}^{m} \omega_{l}^{(i)} x^{(i)}}{\sum_{i=1}^{m} \omega_{l}^{(i)}}
$$

## Applying EM Algorithm to MG: Calculating $\phi$

- Our problem becomes

$$
\begin{array}{ll}
\max & \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \phi_{j} \\
\text { s.t. } & \sum_{j=1}^{k} \phi_{j}=1
\end{array}
$$

- Using the theory of Lagrange multiplier

$$
\phi_{j}=\frac{1}{m} \sum_{i=1}^{m} \omega_{j}^{(i)}
$$

## Applying EM Algorithm to MG: Calculating $\Sigma$

- Minimizing

$$
\begin{aligned}
& \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}\left[\log \left((2 \pi)^{\frac{n}{2}}\left|\Sigma_{j}\right|^{\frac{1}{2}}\right)+\frac{1}{2}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)\right] \\
= & \frac{n \log 2 \pi}{2} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}+\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \left|\Sigma_{j}\right| \\
& +\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)
\end{aligned}
$$

## Applying EM Algorithm to MG: Calculating $\Sigma$ (Contd')

- Minimizing

$$
\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \left|\Sigma_{j}\right|+\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)
$$

- Therefore, we have
$\nabla_{\Sigma_{j}}\left(\sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)} \log \left|\Sigma_{j}\right|+\sum_{i=1}^{m} \sum_{j=1}^{k} \omega_{j}^{(i)}\left(x^{(i)}-\mu_{j}\right)^{T} \Sigma_{j}^{-1}\left(x^{(i)}-\mu_{j}\right)\right)=0$ for $\forall j \in\{1, \cdots, k\}$


## Applying EM Algorithm to MG: Calculating $\Sigma$ (Contd')

- By applying

$$
\begin{aligned}
& \nabla_{X} \operatorname{tr}\left(A X^{-1} B\right)=-\left(X^{-1} B A X^{-1}\right)^{T} \\
& \nabla_{A}|A|=|A|\left(A^{-1}\right)^{T}
\end{aligned}
$$

- We get a solution

$$
\Sigma_{j}=\frac{\sum_{i=1}^{m} \omega_{j}^{(i)}\left(x^{(i)}-\mu_{j}\right)\left(x^{(i)}-\mu_{j}\right)^{T}}{\sum_{i=1}^{m} \omega_{j}^{(i)}}
$$

where $j=1, \cdots, k$

- Check the derivations by yourself!


## Naive Bayes with Missing Labels

- For any $x$, we have

$$
p(x)=\sum_{y=1}^{k} p(x, y)=\sum_{y=1}^{k}\left(p(y) \prod_{j=1}^{n} p_{j}\left(x_{j} \mid y\right)\right)
$$

- The log-likelihood function is then defined as

$$
\ell(\theta)=\sum_{i=1}^{m} \log p\left(x^{(i)}\right)=\sum_{i=1}^{m} \log \sum_{y=1}^{k}\left(p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)\right)
$$

- Maximizing $\ell(\theta)$ subject to the following constraints
- $p(y) \geq 0$ for $\forall y \in\{1, \cdots, k\}$, and $\sum_{y=1}^{k} p(y)=1$
- For $\forall y \in\{1, \cdots, k\}, j \in\{1, \cdots, n\}, x_{j} \in\{0,1\}, p_{j}\left(x_{j} \mid y\right) \geq 0$
- For $\forall y \in\{1, \cdots, k\}$ and $j \in\{1, \cdots, n\}, \sum_{x_{j} \in\{0,1\}} p_{j}\left(x_{j} \mid y\right)=1$


## Naive Bayes with Missing Labels (Contd.)

- When labels are given

$$
\ell(\theta)=\sum_{i=1}^{m} \log \left(p\left(y^{(i)}\right) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y^{(i)}\right)\right)
$$

- When labels are missed

$$
\ell(\theta)=\sum_{i=1}^{m} \log \sum_{y=1}^{k}\left(p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)\right)
$$

## Applying EM Algorithm to Naive Bayes

- Repeat the following steps until convergence
- (E-step) For each $i=1, \cdots, m$ and $y=1, \cdots, k$ set

$$
Q_{i}(y)=p\left(y^{(i)}=y \mid x^{(i)}\right)=\frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)}{\sum_{y^{\prime}=1}^{k} p\left(y^{\prime}\right) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y^{\prime}\right)}
$$

- (M-step) Update the parameters

$$
\begin{aligned}
& p(y)=\frac{1}{m} \sum_{i=1}^{m} Q_{i}(y), \quad \forall y \\
& p_{j}(x \mid y)=\frac{\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)}{\sum_{i=1}^{m} Q_{i}(y)}, \quad \forall x, y
\end{aligned}
$$

## Applying EM Algorithm to NB: E-Step

$$
\begin{aligned}
Q_{i}(y) & =p\left(y \mid x^{(i)}\right) \\
& =\frac{p\left(x^{(i)} \mid y\right) p(y)}{p\left(x^{(i)}\right)} \\
& =\frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)}{\sum_{y^{\prime}=1}^{k} p\left(x^{(i)}, y^{\prime}\right)} \\
& =\frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)}{\sum_{y^{\prime}=1}^{k} p\left(x^{(i)} \mid y^{\prime}\right) p\left(y^{\prime}\right)} \\
& =\frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)}{\sum_{y^{\prime}=1}^{k} p\left(y^{\prime}\right) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y^{\prime}\right)}
\end{aligned}
$$

## Applying EM Algorithm to NB: M-Step

$$
\begin{aligned}
& \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log \frac{p\left(x^{(i)}, z^{(i)}=y\right)}{Q_{i}(y)} \\
= & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log \frac{p\left(x^{(i)} \mid z^{(i)}=y\right) p\left(z^{(i)}=y\right)}{Q_{i}(y)} \\
= & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log \frac{p(y) \prod_{j=1}^{n} p_{j}\left(x_{j}^{(i)} \mid y\right)}{Q_{i}(y)} \\
= & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y)\left[\log p(y)+\sum_{j=1}^{n} \log p_{j}\left(x_{j}^{(i)} \mid y\right)-\log Q_{i}(y)\right] \\
= & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log p(y)+\sum_{i=1}^{m} \sum_{y=1}^{k} \sum_{j=1}^{n} Q_{i}(y) \log p_{j}\left(x_{j}^{(i)} \mid y\right) \\
& -\sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log Q_{i}(y)
\end{aligned}
$$

## Applying EM Algorithm to NB: M-Step (Contd.)

$$
\begin{aligned}
& \sum_{i=1}^{m} \sum_{y=1}^{k} \sum_{j=1}^{n} Q_{i}(y) \log p_{j}\left(x_{j}^{(i)} \mid y\right) \\
= & \sum_{y=1}^{k} \sum_{j=1}^{n}\left(\sum_{i: x_{j}^{(i)}=0} Q_{i}(y)\right) \log p_{j}(x=0 \mid y) \\
& +\sum_{y=1}^{k} \sum_{j=1}^{n}\left(\sum_{i: x_{j}^{(i)}=1} Q_{i}(y)\right) \log p_{j}(x=1 \mid y) \\
= & \sum_{y=1}^{k} \sum_{j=1}^{n} \sum_{x \in\{0,1\}}\left(\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)\right) \log p_{j}(x \mid y)
\end{aligned}
$$

## Applying EM Algorithm to NB: M-Step (Contd.)

$$
\begin{array}{ll}
\max & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log p(y)+\sum_{y=1}^{k} \sum_{j=1}^{n} \sum_{x \in\{0,1\}}\left(\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)\right) \log p_{j}(x \mid y) \\
\text { s.t. } \quad & \sum_{y=1}^{k} p(y)=1 \\
& \sum_{x \in\{0,1\}} p_{j}(x \mid y)=1, \forall y=1, \cdots, k, \forall j=1, \cdots, n \\
& p(y) \geq 0, \forall y=1, \cdots, k \\
& p_{j}(x \mid y) \geq 0, \forall j=1, \cdots, n, \quad \forall x=0,1, \quad \forall y=1, \cdots, k
\end{array}
$$

## Applying EM Algorithm to NB: M-Step (Contd.)

- Problem I

$$
\begin{array}{ll}
\max & \sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y) \log p(y) \\
\text { s.t. } & \sum_{y=1}^{k} p(y)=1 \\
& p(y) \geq 0, \quad \forall y=1, \cdots, k
\end{array}
$$

- Solution (by Lagrange multiplier):

$$
p(y)=\frac{\sum_{i=1}^{m} Q_{i}(y)}{\sum_{i=1}^{m} \sum_{y=1}^{k} Q_{i}(y)}=\frac{1}{m} \sum_{i=1}^{m} Q_{i}(y)
$$

## Applying EM Algorithm to NB: M-Step (Contd.)

- Problem II

$$
\begin{array}{ll}
\max & \sum_{y=1}^{k} \sum_{j=1}^{n} \sum_{x \in\{0,1\}}\left(\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)\right) \log p_{j}(x \mid y) \\
\text { s.t. } & \sum_{x \in\{0,1\}} p_{j}(x \mid y)=1, \forall y=1, \cdots, k, \forall j=1, \cdots, n \\
& p_{j}(x \mid y) \geq 0, \forall j=1, \cdots, n, \quad \forall x=0,1, \quad \forall y=1, \cdots, k
\end{array}
$$

- Solution (by Lagrange multiplier):

$$
p_{j}(x \mid y)=\frac{\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)}{\sum_{x^{\prime} \in\{0,1\}} \sum_{i: x_{j}^{(i)}=x^{\prime}} Q_{i}(y)}=\frac{\sum_{i: x_{j}^{(i)}=x} Q_{i}(y)}{\sum_{i=1}^{m} Q_{i}(y)}
$$

## Thanks!

Q \& A

