Lecture 09: Linear Discriminant Analysis
Introduction to Machine Learning [25737]

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Section 1

Approach Definitions
Discriminant Analysis

Assume we consider the following model for classification:

$$p(y = c | x; \theta) = \frac{p(x | y = c; \theta)p(y = c | \theta)}{\sum_{c'} p(x | y = c'; \theta)p(y = c' | \theta)}$$

where:

- $p(y = c | \theta)$: Prior probability over labels
- $p(x | y = c; \theta)$: Class conditional density

Using special options for class conditional density, we can show that:

$$p(y | x; \theta) = \mathbf{w}^T \mathbf{x} + \text{constant}$$

The resulting model is known as linear discriminant analysis.
Section 2

Gaussian Discriminant Analysis
Gaussian Discriminant Analysis (GDA)

Class Conditional Density

For Gaussian discriminant analysis, the class conditional density is:

\[ p(x|y = c; \theta) = \mathcal{N}(x|\mu_c, \Sigma_c) \]

The above selection result in the following posterior over class labels:

\[ p(y = c|x, \theta) \propto \pi_c \mathcal{N}(x|\mu_c, \Sigma_c) \]

where

\[ \pi_c = p(y = c|\theta) \]

\[ \mathcal{N}(x|\mu_c, \Sigma_c) = \frac{1}{(2\pi)^{d/2}\Sigma_c^{1/2}} \exp \left[ -\frac{1}{2}(y - \mu_c)^T \Sigma_c^{-1}(y - \mu_c) \right] \]
Quadratic Decision Boundary

Consider the log posterior probability as:

$$\log p(y = c | \mathbf{x}; \theta) = \log \pi_c - \frac{1}{2} (\mathbf{x} - \mu_c)^T \Sigma_c^{-1} (\mathbf{x} - \mu_c) + \text{const}$$

This method is called Quadratic Discriminant Analysis (QDA) because the decision boundary is a quadratic function.

Linear Decision Boundary

If we assume $\Sigma = \Sigma_c$, then:

$$\log p(y = c | \mathbf{x}; \theta) = \log \pi_c - \frac{1}{2} \mu_c^T \Sigma^{-1} \mu_c + \mathbf{x}^T \Sigma^{-1} \mu_c + \text{const} - \frac{1}{2} \mathbf{x}^T \Sigma^{-1} \mathbf{x}$$

$$= \gamma_c + \mathbf{x}^T \beta_c + \kappa$$

This method is called Linear Discriminant Analysis (LDA) because the decision boundary is a linear function.
Quadratic vs Linear Discriminant Analysis

(a) QDA

(b) LDA

Figure: Decision boundary comparison
Section 3

Connection Between LDA and MLR
Connection Between LDA and MLR

**Similarity**

As we can see, LDA can be formulated as:

\[ p(y = c|x, \theta) = \frac{\exp(\beta_c^T x + \gamma_c)}{\sum_{c'=1}^C \exp(\beta_{c'}^T x + \gamma_{c'})} = \frac{\exp(w_c^T [1; x])}{\sum_{c'=1}^C \exp(w_{c'}^T [1; x])} \]

Thus the posterior form is similar to MLR.

**Difference**

- In LDA, we first estimate prior probability over labels and class conditional density, and derive \( \{w_c\}_{c=1}^C \) from them.
- In MLR, we estimate \( \{w_c\}_{c=1}^C \) directly to maximize conditional likelihood \( p(y|x, \theta) \).
The likelihood function can be formulated as:

\[
p(D|\theta) = p \left( \{ (x_n, y_n) \}_{n=1}^{N} | \theta \right) = \prod_{n=1}^{N} p(x_n, y_n | \theta) \tag{1}
\]

\[
\prod_{n=1}^{N} p(y_n | \theta) p(x_n | y_n, \theta) = \prod_{n=1}^{N} \text{Cat}(y_n | \pi) \prod_{c=1}^{C} \mathcal{N}(x_n | \mu_c, \Sigma_c) \mathbb{I}(y_n = c) \tag{2}
\]

where we use independency of training samples and probability chain rule for equality (1) and (2), respectively. Note that the parameter vector is:

\[
\theta = [\pi; \mu_1; \ldots; \mu_C; \text{vec}(\Sigma_1); \ldots; \text{vec}(\Sigma_C)]
\]
The likelihood function and its log version are:

\[
p(D|\theta) = \prod_{n=1}^{N} \operatorname{Cat}(y_n|\pi) \prod_{c=1}^{C} \mathcal{N}(x_n|\mu_c, \Sigma_c)^{I(y_n=c)}
\]

\[
\Rightarrow \log p(D|\theta) = \left[ \sum_{n=1}^{N} \sum_{c=1}^{C} I(y_n = c) \log \pi_c \right] + \sum_{c=1}^{C} \left[ \sum_{n:y_n=c} \log \mathcal{N}(x_n|\mu_c, \Sigma_c) \right]
\]

Using differentiation, we can calculate the model parameters as:

\[
\hat{\pi}_c = \frac{N_c}{N}
\]

\[
\hat{\mu}_c = \frac{1}{N_c} \sum_{n:y_n=c} x_n
\]

\[
\hat{\Sigma}_c = \frac{1}{N_c} \sum_{n:y_n=c} (x_n - \hat{\mu}_c)(x_n - \hat{\mu}_c)^T
\]
**Tied Covariance Matrices**

Tied covariance matrices is the situation where we force all covariance matrices to be equal as:

\[ \Sigma_c = \Sigma, \ c = 1, \ldots, C \]

MLE estimation for tied covariance matrix is:

\[
\hat{\Sigma} = \frac{1}{N} \sum_{c=1}^{C} \sum_{n: y_n = c} (x_n - \hat{\mu}_c)(x_n - \hat{\mu}_c)^T
\]

**LDA and Tied Covariance Matrix**

When the covariance matrix is tied, QDA simplifies to LDA.

**Diagonal LDA**

We can simplify tied covariance matrix further by assuming it to be diagonal, so: \( \Sigma_c = D, \ c = 1, \ldots, C \)
Nearest Centroid Classifier

Assume the prior probability over classes is uniform, so:

$$\pi_c = \frac{1}{C}, \ c = 1, \ldots, C$$

If the covariance matrices are tied, then:

$$\hat{y}(x) = \arg\max_c \log p(y = c|x, \theta) = \arg\min_c (x - \mu_c)^T\Sigma^{-1}(x - \mu_c)$$

$$= \arg\min_c \Delta^2_{\Sigma}(x, \mu_c)$$

Thus the class whose mean has minimum Mahalanobis distance to the query point $x$ is selected as the label.
Section 4

Naive Bayes Classifier
Main Assumption

The input features are mutually independent given the class label. In other words:

\[ p(x|y=c, \theta) = \prod_{d=1}^{D} p(x_d|y=c, \theta_{dc}) \]

where \( \theta_{dc} \) is model parameter vector for conditional density for class \( c \) and feature \( d \). The posterior over class label is:

\[ p(y = c|x, \theta) = \frac{p(y = c|\pi) \prod_{d=1}^{D} p(x_d|y = c, \theta_{dc})}{\sum_{c'} p(y = c'|\pi) \prod_{d=1}^{D} p(x_d|y = c', \theta_{dc'})} \]

Pros and cons

- The naive model may not hold in many real world application.
- Naive Bayes model is relatively immune to overfitting.
Example Models

Binary Features
In this case $x_d \in \{0, 1\}$ and thus the class conditional density is:

$$p(x|y = c, \theta) = \prod_{d=1}^{D} \text{Ber}(x_d|\theta_{dc})$$

where $\theta_{dc}$ shows the probability that $x_d = 1$ in class $c$. This model is known as multivariate Bernoulli naive Bayes.

Categorical Features
In this case $x_d \in \{0, 1, \ldots, K\}$ and thus the class conditional density is:

$$p(x|y = c, \theta) = \prod_{d=1}^{D} \text{Cat}(x_d|\theta_{dc})$$

where $\theta_{dck}$ shows the probability that $x_d = k$ in class $c$. 
Real-values Features

In this case \( x_d \in \mathbb{R} \) and thus we can use univariate Gaussian for each dimension in each class. Thus the class conditional density is:

\[
p(x|y = c, \theta) = \prod_{d=1}^{D} \mathcal{N}(x_d|\mu_{dc}, \sigma^2_{dc})
\]

where \( \mu_{dc} \) and \( \sigma^2_{dc} \) shows the mean and variance of feature \( d \) in class \( c \).
Model Fitting

MLE

The likelihood for the dataset $\mathcal{D}$ is:

$$p(\mathcal{D}|\theta) = \prod_{n=1}^{N} p(y_n|\theta)p(x_n|y_n, \theta) \overset{(1)}{=} \prod_{n=1}^{N} p(y_n|\theta) \prod_{d=1}^{D} p(x_{nd}|y_n, \theta_d)$$

$$= \prod_{n=1}^{N} \text{Cat}(y_n|\pi) \prod_{d=1}^{D} \prod_{c=1}^{C} p(x_{nd}|\theta_{dc}) \mathbb{I}(y_n=c)$$

where we use Naive Bayes assumption for equality (1).
MLE (Continue)

\[
\log p(D|\theta) = \log \prod_{n=1}^{N} \left( \prod_{c=1}^{C} \pi_c I(y_n = c) \right) \left( \prod_{d=1}^{D} \prod_{c=1}^{C} p(x_{nd}|\theta_{dc}) I(y_n = c) \right)
\]

\[
= \sum_{n=1}^{N} \left( \log \left( \prod_{c=1}^{C} \pi_c I(y_n = c) \right) + \log \left( \prod_{d=1}^{D} \prod_{c=1}^{C} p(x_{nd}|\theta_{dc}) I(y_n = c) \right) \right)
\]

\[
= \sum_{n=1}^{N} \left( \left[ \sum_{c=1}^{C} \mathbb{I}(y_n = c) \log \pi_c \right] + \left[ \sum_{d=1}^{D} \sum_{c=1}^{C} \mathbb{I}(y_n = c) \log p(x_{nd}|\theta_{dc}) \right] \right)
\]

\[
= \left[ \sum_{n=1}^{N} \sum_{c=1}^{C} \mathbb{I}(y_n = c) \log \pi_c \right] + \left[ \sum_{n=1}^{N} \sum_{d=1}^{D} \sum_{c=1}^{C} \mathbb{I}(y_n = c) \log p(x_{nd}|\theta_{dc}) \right]
\]
MLE for $\pi$

Irrespective of class conditional density, the MLE for $\pi$ is the vector of empirical counts as $\hat{\pi}_c = \frac{N_c}{N}$.

MLE for $\theta_{dc}$

- Binary features: $\hat{\theta}_{dc} = \frac{N_{dc}}{N_c}$
- Categorical features: $\hat{\theta}_{dck} = \frac{N_{dck}}{N_c}$, $k = 1, \ldots, K$
- Real-valued features (Univariate Gaussian):
  
  $$\hat{\mu}_{dc} = \frac{1}{N_c} \sum_{n=1}^{N} \mathbb{I}(y_n = c)x_{nd}$$

  $$\hat{\sigma}_{dc}^2 = \frac{1}{N_c} \sum_{n=1}^{N} \mathbb{I}(y_n = c)(x_{nd} - \hat{\mu}_{dc})^2$$
Section 5

Generative vs. Discriminative
Generative vs. Discriminative

**MLR vs DA**

In MLR, we have $p(y|x; \theta) = \text{Cat}(y|S(W^T x + b))$ and the likelihood is:

$$
p(D|\theta) = p(\{y_n\}_{n=1}^N|\{x_n\}_{n=1}^N, \theta) = \prod_{n=1}^N p(y_n|x_n, \theta)
$$

In Discriminant analysis, we have $p(y = c|x; \theta) = \frac{p(x|y=c;\theta)p(y=c|\theta)}{\sum_{c'} p(x|y=c';\theta)p(y=c'|\theta)}$ and the likelihood is:

$$
p(D|\theta) = p(\{(x_n, y_n)\}_{n=1}^N|\theta) = \prod_{n=1}^N p(x_n, y_n|\theta) = \prod_{n=1}^N p(x_n|y_n, \theta)p(y_n|\theta)
$$
Generative vs. Discriminative

**Discriminative**
By training MLR:
- You have access to $p(y|x, \theta)$ which can be used to generate label for a query input $x$ (discriminate the label of $x$).
- You can’t generate samples from specific class $y = k$.

**Generative**
By training DA:
- You have access to $p(y|x, \theta)$ which can be used to generate label for a query input $x$ (discriminate the label of $x$).
- You have access to $p(x|y, \theta)$ that can be used to generate samples from specific class $y = k$. 