

# Multivariate Methods

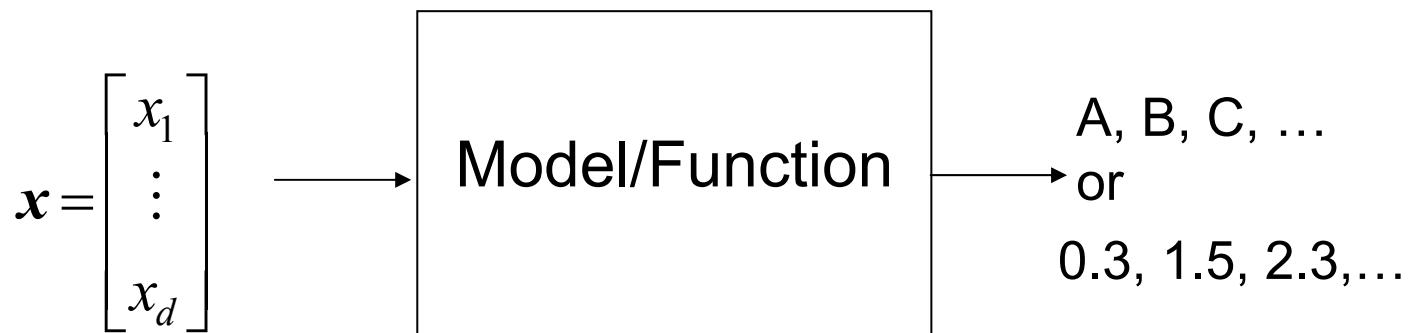
Berlin Chen, 2005

References:

1. *Introduction to Machine Learning* , Chapter 5

# Multivariate Methods

- Input: a data sample with multiple features (variables/inputs)
- Output (of Prediction)
  - Classification: class code (discrete variable)
  - Regression: real number (continuous variable)



- Supervised learning
  - Model/function to be trained with labeled training samples

# Multivariate Data

- Each data sample is represented by an observation vector with  $d$  dimensions
  - Each dimension of the vector is termed input/feature/attribute
  - Dimensions with different types and value domains
- The whole data set of size  $N$  can be viewed as a data matrix

$$\mathbf{X} = \begin{bmatrix} X_1^1 & X_2^1 & \cdots & X_d^1 \\ X_1^2 & X_2^2 & \cdots & X_d^2 \\ \vdots & \vdots & \vdots & \vdots \\ X_1^N & X_2^N & \cdots & X_d^N \end{bmatrix}$$

samples/instances/items

Inputs/features/attributes

Reduced to a naïve Bayes' classifier

- Features are usually assumed correlated !
$$P(\mathbf{x}|C_i) = P(x_1, x_2, \dots, x_d | C_i) = \prod_{j=1}^d P(x_j | C_i)$$
- Otherwise, there is no need for a multivariate analysis

# Multivariate Data (cont.)

- Motivations for multivariate data analysis
  - Simplification
    - Assume that the large body of data can be well summarized by means of relatively few parameters
  - Exploration
    - Predict the value of one variable from the values of other variables
      - Multivariate classification (Discrete)
      - Multivariate regression (Numeric)

# Parameter Estimation

- Mean of data samples

$$E[\mathbf{X}] = \int \mathbf{x} \cdot P(\mathbf{x}) d\mathbf{x} = \boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_d \end{bmatrix}$$

Mean of Column 1 of matrix  $\mathbf{X}$   
 Mean of Column  $d$  of matrix  $\mathbf{X}$

- Covariance matrix of data samples

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \dots & \sigma_{2d} \\ \vdots & \vdots & \vdots & \vdots \\ \sigma_{d1} & \dots & \dots & \sigma_d^2 \end{bmatrix}$$

$\sigma_i^2$  : variance of a variable  $X_i$

$\sigma_{ij}$  : covariance of two variables  $X_i$  and  $X_j$

$$\begin{aligned} \sigma_{ij} &\equiv \text{Cov}(X_i, X_j) \\ &= E[(X_i - \mu_i)(X_j - \mu_j)] = E[X_i X_j] - \mu_i \mu_j \end{aligned}$$

$E[X_i X_j] = E[X_i] E[X_j] = \mu_i \mu_j$   
 if  $X_i$  and  $X_j$  are independent  
 $= E[(X_i - \mu_i)^2] = E[X_i^2] - (\mu_i)^2$   
 $= \sigma_i^2$

# Parameter Estimation (cont.)

- Covariance matrix is symmetric
  - Diagonal terms: variances
  - Off-diagonal terms: covariances

$$\Sigma = \text{Cov}(X) = E[(X - \mu)(X - \mu)^T] = E[XX^T] - \mu\mu^T$$

- Correlation between two variables  $X_i$  and  $X_j$

$$\text{Corr}(X_i, X_j) = \frac{\sigma_{ij}}{\sigma_i \sigma_j}, \quad -1 \leq \text{Corr}(X_i, X_j) \leq 1$$

independent  $\rightarrow$  uncorrelated

- Two variables independent  $\rightarrow$  covariance =correlation=0
- But covariance =correlation=0 does not imply two variables are independent (nonlinear dependence)

# Parameter Estimation (cont.)

- If  $X_i$  and  $X_j$  are linear dependent

$$X_j = a \cdot X_i + b \quad (a > 0)$$

$$\Rightarrow E[X_j] = \mu_j = a \cdot [X_i] + b = a \cdot \mu_i + b$$

$$\sigma_j^2 = \text{var}(X_j) = E[(X_j - \mu_j)^2] = a^2 \cdot \text{var}(X_i) = a^2 \cdot \sigma_i^2$$

$$\sigma_{ij} = E[(X_i - \mu_i)(X_j - \mu_j)] = E[(X_i - \mu_i)((a \cdot X_i + b) - (a \cdot \mu_i + b))] = a \cdot E[(X_j - \mu_j)^2] = a \cdot \sigma_i^2$$

$$\Rightarrow \rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j} = \frac{a \cdot \sigma_i^2}{\sigma_i \cdot (a \cdot \sigma_i)} = 1$$

Similarly, for

$$X_j = -a \cdot X_i + b \quad (a > 0)$$

$$\rho_{ij} = -1$$

# Parameter Estimation (cont.)

- Maximum Likelihood Estimators

- Sample mean as an estimator for mean

$$\bar{\mu} = \mathbf{m} = \frac{\sum_{t=1}^N \mathbf{x}^t}{N} \text{ with } m_i = \frac{\sum_{t=1}^N x_i^t}{N}, i=1,\dots,d$$

- Sample covariance matrix as an estimator for covariance matrix

$$s_i^2 = \frac{\sum_{t=1}^N (x_i^t - m_i)^2}{N}$$

$$s_{ij} = \frac{\sum_{t=1}^N (x_i^t - m_i)(x_j^t - m_j)}{N}$$

$$\bar{\Sigma} = \mathbf{C} = \begin{bmatrix} s_1^2 & s_{12} & \cdots & s_{1d} \\ s_{21} & s_2^2 & \cdots & s_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ s_{d1} & \cdots & \cdots & s_d^2 \end{bmatrix}$$

- Sample correlation coefficients

$$r_{ij} = \frac{s_{ij}}{s_i s_j}$$

# Multivariate Normal Distribution

- A random variable  $x$  that is  $d$ -dimensional and normal distributed, is denoted as  $x \sim N_d(\mu, \Sigma)$

$$P(x) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu)\right]$$

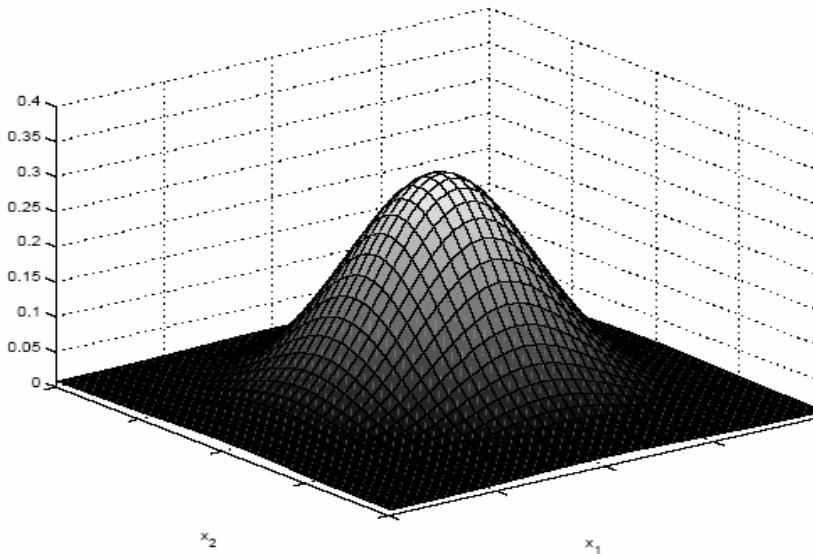
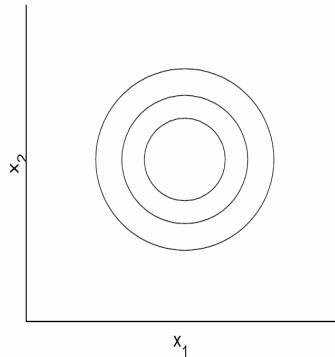


Figure 5.1: Bivariate normal distribution.

# Multivariate Normal Distribution (cont.)

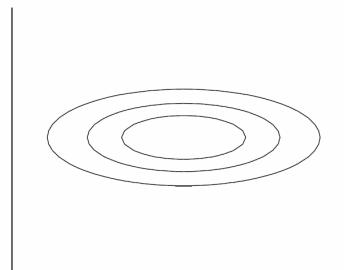
- If each dimension is independent of one another and with same variance value

$$\text{Cov}(x_1, x_2) = 0, \text{Var}(x_1) = \text{Var}(x_2)$$



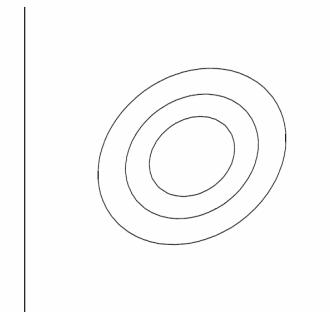
- If each dimension is independent of one another and with different variance value

$$\text{Cov}(x_1, x_2) = 0, \text{Var}(x_1) > \text{Var}(x_2)$$



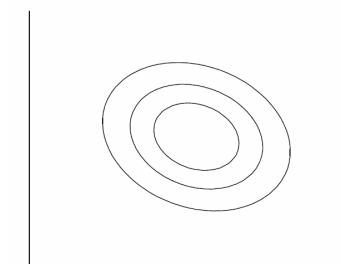
- If each dimension is dependent of one another with  $\text{Corr}(X_1, X_2) > 0$

$$\text{Cov}(x_1, x_2) > 0$$



- If each dimension is dependent of one another with  $\text{Corr}(X_1, X_2) < 0$

$$\text{Cov}(x_1, x_2) < 0$$



# Multivariate Normal Distribution (cont.)

- If the components of random variable  $x$  are independent

$$\begin{aligned} P(x) &= P(x_1, \dots, x_j, \dots, x_d) = \prod_{j=1}^d P(x_j) \\ &= \frac{1}{(2\pi)^{d/2} \prod_{j=1}^d \sigma_j} \exp \left[ -\frac{1}{2} \sum_{j=1}^d \left( \frac{x_j - \mu_j}{\sigma_j} \right)^2 \right] \end{aligned}$$

Also note that  $P(x_j) = \frac{1}{(2\pi)^{1/2} \sigma_j} \exp \left[ -\frac{1}{2} \left( \frac{x_j - \mu_j}{\sigma_j} \right)^2 \right]$

# Multivariate Normal Distribution (cont.)

- Recall: The project of a  $d$ -dimensional normal distribution on a vector  $\mathbf{w}$  is univariate normal (suppose that  $\|\mathbf{w}\|=1$ )

$$\mathbf{w}^T \mathbf{x} = w_1 x_1 + w_2 x_2 + \cdots + w_d x_d \sim N(\mathbf{w}^T \boldsymbol{\mu}, \mathbf{w}^T \boldsymbol{\Sigma} \mathbf{w})$$

$$E[\mathbf{w}^T \mathbf{x}] = \mathbf{w}^T E[\mathbf{x}] = \frac{\mathbf{w}^T \boldsymbol{\mu}}{\text{scalar}}$$

$$\begin{aligned} \text{Var}(\mathbf{w}^T \mathbf{x}) &= E[(\mathbf{w}^T \mathbf{x} - \mathbf{w}^T \boldsymbol{\mu})(\mathbf{w}^T \mathbf{x} - \mathbf{w}^T \boldsymbol{\mu})^T] \\ &= E[\mathbf{w}^T (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{w}] = \mathbf{w}^T E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T] \mathbf{w} = \frac{\mathbf{w}^T \boldsymbol{\Sigma} \mathbf{w}}{\text{scalar}} \end{aligned}$$

- The project of a  $d$ -dimensional normal distribution to a  $k$ -dimensional space is  $k$ -variate normal

$$\mathbf{W}^T \mathbf{x} \sim N_k \left( \underbrace{\mathbf{W}^T \boldsymbol{\mu}}_{\substack{k\text{-dim} \\ \text{vector}}}, \underbrace{\mathbf{W}^T \boldsymbol{\Sigma} \mathbf{W}}_{\substack{k \times k \\ \text{matrix}}} \right) \quad \mathbf{W} = [\mathbf{w}_1 \quad \mathbf{w}_2 \quad \cdots \quad \mathbf{w}_k]$$

# Multivariate Classification

- Normal density  $N_d(\boldsymbol{\mu}_i, \Sigma_i)$  as the class-conditional probability  $P(x|C_i)$  of random variable  $x \in \Re^d$

$$P(x|C_i) = \frac{1}{(2\pi)^{d/2} |\Sigma_i|^{1/2}} \exp \left[ -\frac{1}{2} (x - \boldsymbol{\mu}_i)^T \Sigma_i^{-1} (x - \boldsymbol{\mu}_i) \right]$$

- Define the discriminant function as

$$\begin{aligned} g_i(x) &= \log P(x|C_i) + \log P(C_i) \\ &= -\frac{d}{2} \log 2\pi - \frac{1}{2} \log |\Sigma_i| - \frac{1}{2} (x - \boldsymbol{\mu}_i)^T \Sigma_i^{-1} (x - \boldsymbol{\mu}_i) + \log P(C_i) \end{aligned}$$

# Multivariate Classification (cont.)

- Maximum likelihood (ML) training of classifiers
  - Given a set of labeled samples

$$X = \{x^t, r^t\}, r_i^t = 1 \text{ if } x^t \in C_i \text{ and } 0 \text{ otherwise}$$

$$\hat{P}(C_i) = \frac{\sum_{t=1}^N r_i^t}{N}$$

$$\hat{\mu}_i = \mathbf{m}_i \text{ (sample mean)} = \frac{\sum_{t=1}^N r_i^t \mathbf{x}^t}{\sum_{t=1}^N r_i^t}$$

$$\hat{\Sigma}_i = \mathbf{S}_i \text{ (sample covariance matrix)} = \frac{\sum_{t=1}^N r_i^t (\mathbf{x}^t - \mathbf{m}_i)(\mathbf{x}^t - \mathbf{m}_i)^T}{\sum_{t=1}^N r_i^t}$$

# Quadratic Discriminant

- The discriminant function with normal class-conditional density can be expressed as a **quadratic discriminant**

$$\begin{aligned}g_i(\mathbf{x}) &= \log P(\mathbf{x}|C_i) + \log P(C_i) \\&= -\frac{d}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{S}_i| - \frac{1}{2} (\mathbf{x} - \mathbf{m}_i)^T \mathbf{S}_i^{-1} (\mathbf{x} - \mathbf{m}_i) + \log P(C_i) \\&= -\frac{1}{2} (\mathbf{x}^T \mathbf{S}_i^{-1} \mathbf{x} - 2\mathbf{x}^T \mathbf{S}_i^{-1} \mathbf{m}_i + \mathbf{m}_i^T \mathbf{S}_i^{-1} \mathbf{m}_i) - \frac{d}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{S}_i| + \log P(C_i) \\&= \mathbf{x}^T \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^T \mathbf{x} + w_{i0}\end{aligned}$$

quadratic discriminant

$$\mathbf{W}_i = -\frac{1}{2} \mathbf{S}_i^{-1}$$

Recall : second - order polynomial for scalar variable

$$g_i(x) = w_{i2}x^2 + w_{i1}x + w_{i0}$$

$$\mathbf{w}_i = \mathbf{S}_i^{-1} \mathbf{m}_i$$

$$w_{i0} = -\frac{d}{2} \log 2\pi - \frac{1}{2} \mathbf{m}_i^T \mathbf{S}_i^{-1} \mathbf{m}_i - \frac{1}{2} \log |\mathbf{S}_i| + \log P(C_i)$$

# Quadratic Discriminant (cont.)

$$\begin{aligned}g_1(\mathbf{x}) &= \mathbf{x}^T \mathbf{W}_1 \mathbf{x} + \mathbf{w}_1^T \mathbf{x} + w_{10} \\g_2(\mathbf{x}) &= \mathbf{x}^T \mathbf{W}_2 \mathbf{x} + \mathbf{w}_2^T \mathbf{x} + w_{20} \\\tilde{g}(\mathbf{x}) &= g_1(\mathbf{x}) - g_2(\mathbf{x}) \\&= \mathbf{x}^T (\mathbf{W}_1 - \mathbf{W}_2) \mathbf{x} + (\mathbf{w}_1^T - \mathbf{w}_2^T) \mathbf{x} \\&\quad + (w_{10} - w_{20}) \\&= \mathbf{x}^T \mathbf{W}' \mathbf{x} + \mathbf{w}' \mathbf{x} + w'_0\end{aligned}$$

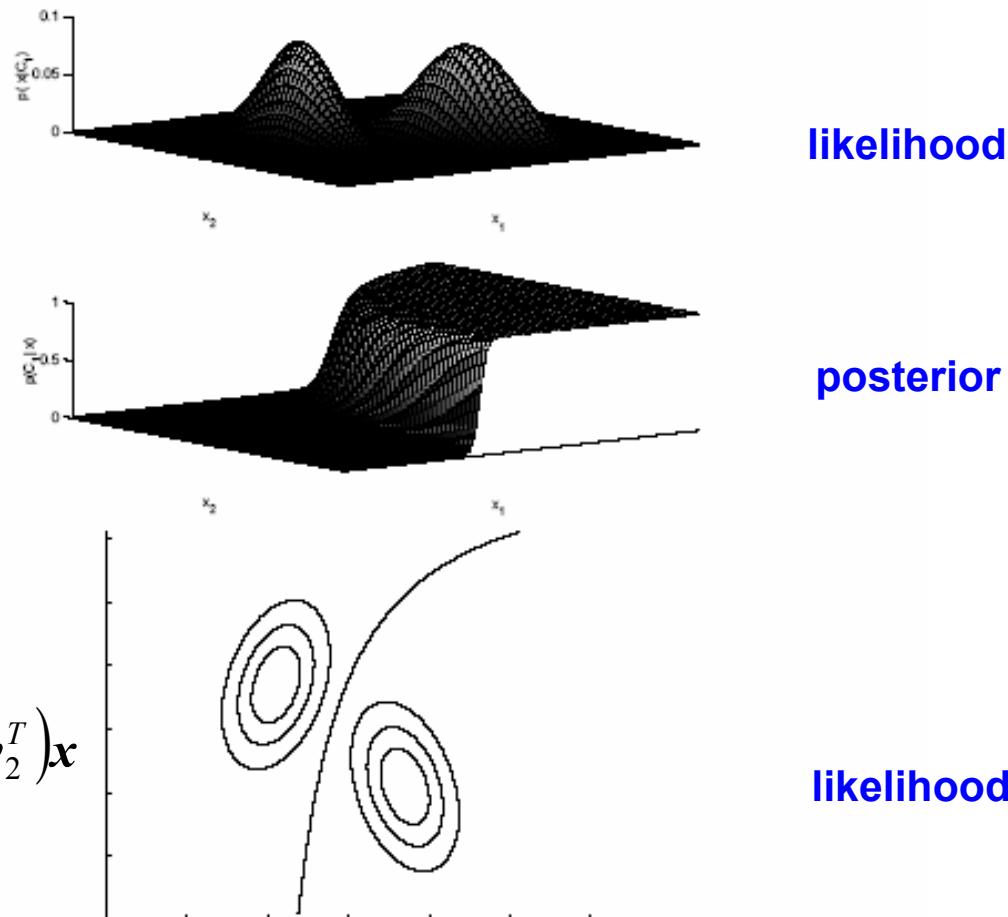


Figure 5.3: Classes have different covariance matrices.

# Linear Discriminant

- The discriminant function with normal class-conditional density **sharing the same covariance matrix** can be expressed as a **linear discriminant**

$$\mathbf{S} = \sum_{i=1}^K \hat{P}(C_i) \cdot \mathbf{S}_i \quad \text{All classes share the same covariance matrix}$$

$$g_i(\mathbf{x}) = \log P(\mathbf{x}|C_i) + \log P(C_i)$$

$$= -\frac{1}{2} (\mathbf{x}^T \mathbf{S}^{-1} \mathbf{x} - 2 \mathbf{x}^T \mathbf{S}^{-1} \mathbf{m}_i + \mathbf{m}_i^T \mathbf{S}^{-1} \mathbf{m}_i) - \frac{d}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{S}| + \log P(C_i)$$

$$\Rightarrow \tilde{g}_i(\mathbf{x}) = \mathbf{w}_i^T \mathbf{x} + w_{i0}$$

$$\mathbf{w}_i = \mathbf{S}^{-1} \mathbf{m}_i$$

$$w_{i0} = -\frac{d}{2} \log 2\pi - \frac{1}{2} \mathbf{m}_i^T \mathbf{S}^{-1} \mathbf{m}_i - \frac{1}{2} \log |\mathbf{S}| + \log P(C_i)$$

# Linear Discriminant (cont.)

covariances (off-diagonal terms of covariance matrix) are not equal to zero

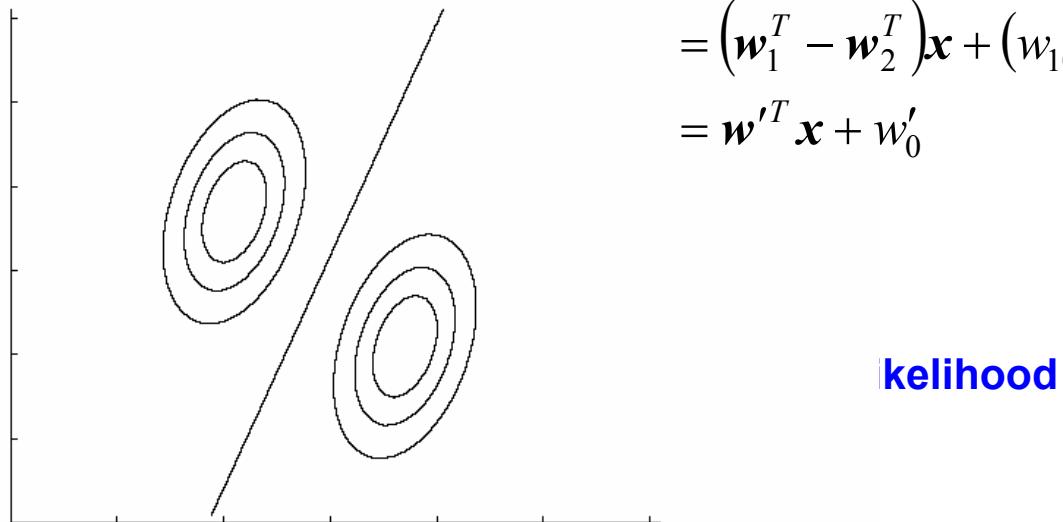


Figure 5.4: Covariances may be arbitrary but shared by both classes.

# Naïve Bayes' Classifier

- The discriminant function with normal class-conditional density sharing the same diagonal covariance matrix can be expressed as a naïve Bayes' classifier

$$g_i(\mathbf{x}) = -\frac{1}{2} \sum_{j=1}^d \left( \frac{x_j - m_{ij}}{s_j} \right)^2 + \log P(C_i)$$

variances (diagonal terms of covariance matrix) are not equal

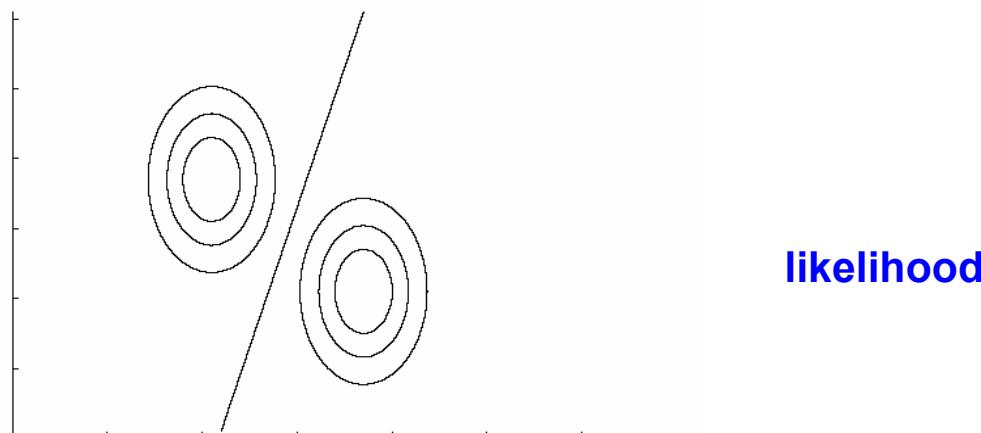


Figure 5.5: All classes have equal, diagonal covariance matrices but variances are not equal.

# Naïve Bayes' Classifier (cont.)

- If the variances (diagonal terms) of the naïve Bayes' classifier are further set to equal for all dimensions

$$g_i(\mathbf{x}) = -\frac{1}{2s^2} \sum_{j=1}^d (x_j - m_{ij})^2 + \log P(C_i)$$

The Mahalanobis distance is reduced to Euclidean distance.  
(all variables/features have the same variance and are independent)

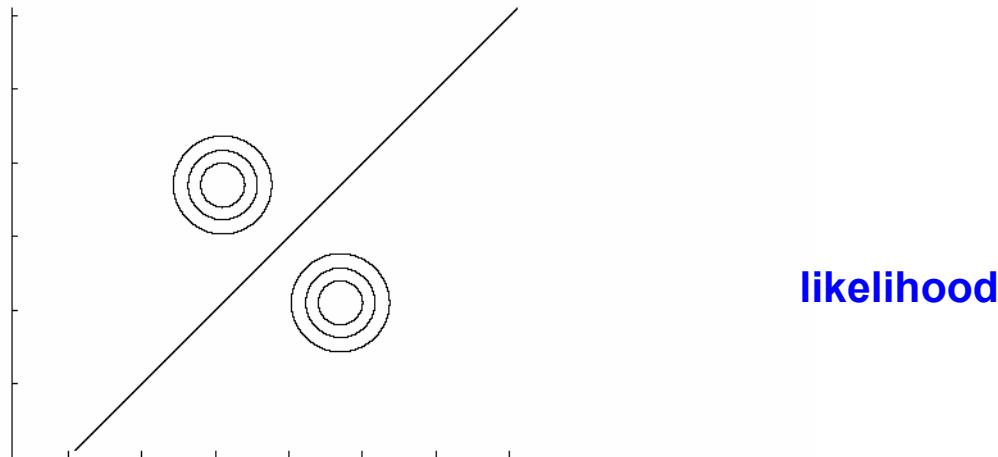


Figure 5.6: All classes have equal, diagonal covariance matrices of equal variances on both dimensions.

# Nearest Mean Classifier

- Assign the data sample to the class of the nearest mean
  - If the priors  $P(C_i)$  are further set to equal

$$\begin{aligned}g_i(\mathbf{x}) &= -\sum_{j=1}^d (x_j - m_{ij})^2 = -\|\mathbf{x} - \mathbf{m}_i\|^2 \\&= -(\mathbf{x} - \mathbf{m}_i)^T (\mathbf{x} - \mathbf{m}_i) \\&= -\left(\mathbf{x}^T \mathbf{x} - 2\mathbf{m}_i^T \mathbf{x} + \mathbf{m}_i^T \mathbf{m}_i\right) \\ \Rightarrow \bar{g}_i(\mathbf{x}) &= \mathbf{m}_i^T \mathbf{x} - \frac{1}{2} \mathbf{m}_i^T \mathbf{m}_i \\&= \mathbf{w}_i^T \mathbf{x} + w_{i0}\end{aligned}$$

where  $\mathbf{w}_i = \mathbf{m}_i$

$$w_{i0} = -\frac{1}{2} \mathbf{m}_i^T \mathbf{m}_i = -\frac{1}{2} \|\mathbf{m}_i\|^2$$

# Tuning Complexity

- Tradeoff between the bias and variance of an estimator

Table 5.1 Reducing variance through simplifying assumptions.

Assumption	Covariance matrix	No. of parameters
Shared, Hyperspheric	$S_i = S = s^2 I$	1
Shared, Axis-aligned	$S_i = S$ , with $s_{ij} = 0$	$d$
Shared, Hyperellipsoidal	$S_i = S$	$d(d + 1)/2$
Different, Hyperellipsoidal	$S_i$	$K \cdot (d(d + 1)/2)$

- Simplifying covariance matrix → decreasing number of parameters → introducing estimation bias
  - Arbitrary covariance matrix → much more data is needed → introducing estimation variance
- Regularized Discriminant Analysis (RDA, 1989)
  - Use a weighted average of three special cases of covariance matrix
 
$$S' = \alpha \cdot \underline{\sigma^2 I} + \beta \cdot \underline{S} + (1 - \alpha - \beta) \cdot \underline{S_i}$$

a shared diagonal covariance matrix (with equal variance) for all classes	a shared covariance matrix for all classes	a specific covariance matrix for each class
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# Discrete Features

- Features that take one of  $n$  different values
  - E.g. pixel  $\in \{\text{on, off}\}$ ; color  $\in \{\text{red, blue, green, black}\}$
- If each feature is a binary random variable  $x_j^t$  ( $x_j^t = 1$  or  $x_j^t = 0$ )
  - Bernoulli distribution
$$P_{ij} = P(x_j^t = 1 | C_i) \quad 1 - P_{ij} = P(x_j^t = 0 | C_i) \Rightarrow P(x_j^t | C_i) = (P_{ij})^{x_j^t} (1 - P_{ij})^{(1-x_j^t)}$$
  - If features are further assumed to be independent
    - Assumption for Naïve Bayes' classifier  $\mathbf{x}^t = \{x_1^t, \dots, x_d^t\}$
$$P(\mathbf{x}^t | C_i) = P(x_1^t, \dots, x_d^t | C_i) = \prod_{j=1}^d P(x_j^t | C_i) = \prod_{j=1}^d (P_{ij})^{x_j^t} (1 - P_{ij})^{(1-x_j^t)}$$
    - Discriminant function

$$g_i(\mathbf{x}^t) = \log P(\mathbf{x}^t | C_i) + \log P(C_i) = \sum_{j=1}^d [x_j^t \log P_{ij} + (1 - x_j^t) \log (1 - P_{ij})] + \log P(C_i)$$

– Linear ?

# Discrete Features (cont.)

- Appendix A

$$\begin{aligned}g_i(\mathbf{x}^t) &= \sum_{j=1}^d \left[ x_j^t \log P_{ij} + (1-x_j^t) \log(1-P_{ij}) \right] + \log P(C_i) \\&= \left[ \sum_{j=1}^d x_j^t \log P_{ij} \right] - \left[ \sum_{j=1}^d x_j^t (1 - \log P_{ij}) \right] + \left[ \sum_{j=1}^d (1 - \log P_{ij}) \right] + \log P(C_i) \\&= \left[ \sum_{j=1}^d x_j^t (2 \cdot (\log P_{ij}) - 1) \right] + \left[ \sum_{j=1}^d (1 - \log P_{ij}) \right] + \log P(C_i) \\&= \mathbf{w}_i^T \mathbf{x}^t + D_i \quad \text{Linear}\end{aligned}$$

where

$$\mathbf{w}_i = \begin{bmatrix} 2 \cdot (\log P_{i1}) - 1 \\ 2 \cdot (\log P_{i2}) - 1 \\ \vdots \\ 2 \cdot (\log P_{id}) - 1 \end{bmatrix} \quad D_i = \left[ \sum_{j=1}^d (1 - \log P_{ij}) \right] + \log P(C_i)$$

# Discrete Features (cont.)

- Maximum likelihood estimation for  $P_{ij}$  (for binary variable)

$$\hat{P}_{ij} = \frac{\sum_{t=1}^N x_j^t \cdot r_i^t}{\sum_{t=1}^N r_i^t}$$

- Extension: features are independent **multinomial random variables**

$$x_j^t \in \{v_{j1}, \dots, v_{jk}, \dots, v_{jn_j}\} \quad z_{jk}^t = \begin{cases} 1 & \text{if } x_j^t = v_{jk} \\ 0 & \text{otherwise} \end{cases}$$

- Define the probability that  $x_j^t$  belongs to  $C_i$  and take  $v_{jk}$  :

$$P_{ijk} = P(z_{jk}^t = 1 | C_i) = P(x_j^t = v_{jk} | C_i) \Rightarrow \prod_{j=1}^d P(x_j^t | C_i) = \prod_{k=1}^{n_j} P_{ijk}^{z_{jk}^t}$$

# Discrete Features (cont.)

- Assumption for Naïve Bayes' classifier

$$P(\mathbf{x}^t | C_i) = P(x_1^t, \dots, x_d^t | C_i) = \prod_{j=1}^d P(x_j^t | C_i) = \prod_{j=1}^d \prod_{k=1}^{n_j} P_{ijk}^{z_{jk}^t}$$

- Discriminant function

$$g_i(\mathbf{x}^t) = \log P(\mathbf{x}^t | C_i) + \log P(C_i) = \sum_{j=1}^d \sum_{k=1}^{n_j} z_{jk}^t \log P_{ijk} + \log P(C_i)$$

- Linear ?

- Maximum likelihood estimation for  $P_{ijk}$

$$\hat{P}_{ijk} = \frac{\sum_{t=1}^N z_{jk}^t \cdot r_i^t}{\sum_{t=1}^N r_i^t}$$