18794 Pattern Recognition Theory Prof. Marios Savvides

HMW-Alexander

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1 Introduction

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2 Decision Theory

2.1 Terms

- Feature Space:
 - Feature: a distinctive characteristic or quality of the object
 - Feature vector: combine more than one feature as a vector
 - Feature space: The space defined by the feature vectors
- Classifiers:
 - **Decision regions**: a classifier partitions the feature space into class-corresponding decision regions.
 - **Decision boundaries**: the borders between the decision regions.

2.2 Bayes Rule

$$P(w_i|x) = \frac{P(x,w_i)}{P(x)} = \frac{P(x|w_i)P(w_i)}{\sum_{k=1}^{C} P(x|w_k)P(w_k)}$$
(1)

- Posterior Probability $P(w_i|x)$: the conditional probability of correct class being w_i given that feature value x has been observed.
- Evidence P(x): the total probability of observing the feature value of x.
- **Likelihood** $P(x|w_i)$: the conditional probability of observing a feature value of x given that the correct class is w_i .
- **Prior Probability** $P(w_i)$: the probability of class w_i , $\sum_{k=1}^{C} P(w_k) = 1$.
- Bayes Classifiers decide on the class that has the largest posterior probability $(\max_{w_i} P(w_i|x))$. They are statistically the best classifiers i.e. they are minimum error classifiers (optimal).

2.3 Minimum Probability of Error

- $\epsilon = P(error|class)$: probability of assigning x to the wrong class w.
- $P_e = \sum_{k=1}^{C} P(w_k) \epsilon_k$: total probability of error.

For the two class case shown above, we want to minimize P_e as below:

$$P_{e} = P(w_{1})\epsilon_{1} + P(w_{2})\epsilon_{2}$$

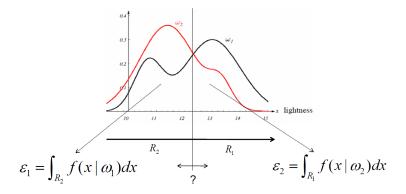
$$= P(w_{1})\int_{R_{2}} f(x|w_{1})dx + P(w_{2})\int_{R_{1}} f(x|w_{2})dx$$

$$= P(w_{1})(1 - \int_{R_{1}} f(x|w_{1})dx) + P(w_{2})\int_{R_{1}} f(x|w_{2})dx$$

$$= P(w_{1}) + \int_{R_{1}} (P(w_{2})f(x|w_{2}) - P(w_{1})f(x|w_{1}))dx$$
(2)

To minimize P_e , we want $P(w_2)f(x|w_2) - P(w_1)f(x|w_1)$ to be always negative (< 0) in the region R_1 :

$$P(w_1)f(x|w_1) - P(w_2)f(x|w_2) > 0 \Rightarrow w_1 P(w_1)f(x|w_1) - P(w_2)f(x|w_2) < 0 \Rightarrow w_2$$
(3)



2.4 Likelihood Ratio

• Likelihood ratio: $l(x) = \frac{f(x|w_1)}{f(x|w_2)}$

• Log likelihood ratio: $\ln(l(x)) = \ln(\frac{f(x|w_1)}{f(x|w_2)}) = \ln(f(x|w_1)) - \ln(f(x|w_2))$

• Ratio of a priori probabilities: $T = \frac{P(w_2)}{P(w_1)}$

• Log ratio of a priori probabilities: $\ln(T) = \ln(\frac{P(w_2)}{P(w_1)}) = \ln(P(w_2)) - \ln(P(w_1))$

$$\ln(l(x)) = \ln(\frac{f(x|w_1)}{f(x|w_2)}) > \ln(\frac{P(w_2)}{P(w_1)}) = \ln(T) \quad \Rightarrow \quad w_1$$

$$\ln(l(x)) = \ln(\frac{f(x|w_1)}{f(x|w_2)}) < \ln(\frac{P(w_2)}{P(w_1)}) = \ln(T) \quad \Rightarrow \quad w_2$$
(4)

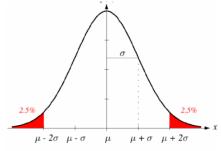
2.4.1 Likelihood as Gaussian distribution

Assume likelihood $f(x|w_i)$ are Gaussian distributions with mean μ_i and variance σ_i^2 .

$$f(x|w_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(x-\mu_i)^2}{2\sigma_i^2}\right)$$
 (5)

The log likelihood ratio:

$$f(x \mid \omega_i)$$



$$\ln(l(x)) = \ln\left(\frac{\frac{1}{\sqrt{2\pi\sigma_1^2}}\exp\left(-\frac{(x-\mu_1)^2}{2\sigma_1^2}\right)}{\frac{1}{\sqrt{2\pi\sigma_2^2}}\exp\left(-\frac{(x-\mu_2)^2}{2\sigma_2^2}\right)}\right)$$

$$= \ln(\frac{\sigma_2}{\sigma_1}) + \frac{(x-\mu_2)^2}{2\sigma_2^2} - \frac{(x-\mu_1)^2}{2\sigma_2^2}$$
(6)

Case: $\sigma_1 = \sigma_2 = \sigma$

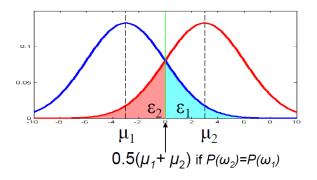
$$\ln(l(x)) = \frac{2x(\mu_1 - \mu_2) - (\mu_1^2 - \mu_2^2)}{2\sigma^2} \tag{7}$$

$$x(\mu_{1} - \mu_{2}) - \frac{\mu_{1}^{2} - \mu_{2}^{2}}{2} > \sigma^{2} \ln(\frac{P(w_{2})}{P(w_{1})}) \Rightarrow w_{1}$$

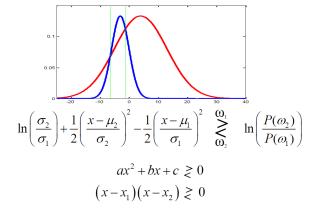
$$x(\mu_{1} - \mu_{2}) - \frac{\mu_{1}^{2} - \mu_{2}^{2}}{2} < \sigma^{2} \ln(\frac{P(w_{2})}{P(w_{1})}) \Rightarrow w_{2}$$
(8)

If $P(w_1) = P(w_2)$

$$x = \frac{\mu_1 + \mu_2}{2} \tag{9}$$



Case: $\sigma_1 \neq \sigma_2$



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3 Parametric & Non-Parametric Density Estimation

Learning & Classification

- Supervised:
 - Bayes Density:
 - * Parametric: assumes a particular form of a PDF (e.g. Gaussian) is known \rightarrow determine the parameters (e.g. mean and variance)

- · Maximum Likelihood $(f(x|w_i))$ Estimation (MLE)
- · Maximum A Posteriori (Bayesian $p(w_i|x)$) Estimation (MAPE)
- * Non-Parametric: no assumption about the density
 - · Parzen Windows
 - · Kernel Density Estimation
 - · K-Nearest Neighbor Rule
- Discriminant Analysis:
 - * Linear
 - * Non-Linear
- Unsupervised:
 - Clustering

3.1 ML Estimation (MLE)

Steps:

- Assume P(x|w) has a known parametric form uniquely determined by the parameter vector θ
- The parameters are assumed to be fixed (i.e. non random) but unknown
- Suppose we have a dataset D with the samples in D having been drawn **independently** according to the probability law P(x|w)
- The MLE is the value of θ that best explains the data and once we know this value, we know P(x|w)

$$\hat{\theta} = \arg\max_{\theta} \{P(D|\theta)\} = \arg\max_{\theta} \{\prod_{k=1}^{N} P(x_k|\theta)\} = \arg\max_{\theta} \{\sum_{k=1}^{N} \log(P(x_k|\theta))\}$$
(10)

Choose the value of θ that is the most likely to give rise to the data we observe.

Method:

- Assume $\theta = [\theta_1, \theta_2, \dots, \theta_p]^T$
- Assume gradient operator $\nabla_{\theta} = [\frac{\partial}{\partial \theta_1}, \frac{\partial}{\partial \theta_2}, \dots, \frac{\partial}{\partial \theta_p}]^T$
- Assume the log-likelihood of the objective function $l(\theta) = \sum_{k=1}^{N} \log(P(x_k|\theta))$
- Therefore: $\nabla_{\theta} l(\theta) = \sum_{k=1}^{N} \nabla_{\theta} \log(P(x_k | \theta)) = 0$

3.1.1 E.g. Univariate Gaussian

$$P(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(x-\mu)^2}{2\sigma^2})$$
 (11)

$$\theta = \begin{bmatrix} \theta_1 = \mu \\ \theta_2 = \sigma^2 \end{bmatrix} \tag{12}$$

$$\log(P(x_k|\theta)) = \log(\frac{1}{\sqrt{2\pi\theta_2}} \exp(-\frac{(x_k - \theta_1)^2}{2\theta_2}))$$

$$= -\frac{1}{2} \log(2\pi\theta_2) - \frac{(x_k - \theta_1)^2}{2\theta_2}$$
(13)

$$\nabla_{\theta} \log(P(x_{k}|\theta)) = \begin{bmatrix} \frac{x_{k} - \theta_{1}}{\theta_{2}} \\ -\frac{1}{2\theta_{2}} + \frac{(x_{k} - \theta_{1})^{2}}{2\theta_{2}} \end{bmatrix}$$

$$\Rightarrow \begin{cases} \sum_{k=1}^{n} \frac{1}{\theta_{2}} (x_{k} - \theta_{1}) = 0 \\ -\sum_{k=1}^{n} \frac{1}{\theta_{2}} + \sum_{k=1}^{n} \frac{(x_{k} - \theta_{1})^{2}}{\theta_{2}^{2}} = 0 \end{cases} \Rightarrow \begin{cases} \hat{\mu} = \frac{1}{n} \sum_{k=1}^{n} x_{k} \\ \hat{\sigma}^{2} = \frac{1}{n} \sum_{k=1}^{n} (x_{k} - \hat{\mu})^{2} \end{cases}$$
(14)

3.1.2 E.g. Multivariate Gaussian

$$P(x|\mu, \Sigma) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu))$$
(15)

Case: only the mean μ is unknown

$$\log(P(x_k|\mu)) = -\frac{1}{2}\log((2\pi)^d|\Sigma|) - \frac{1}{2}(x_k - \mu)^T \Sigma^{-1}(x_k - \mu)$$
(16)

$$\nabla_{\theta} \log(P(x_k|\mu)) = \Sigma^{-1}(x_k - \mu)$$

$$\Rightarrow \sum_{k=1}^{n} \Sigma^{-1}(x_k - \mu) = 0 \Rightarrow \hat{\mu} = \frac{1}{n} \sum_{k=1}^{n} x_k$$
(17)

Case: Neither the mean μ nor the covariance matrix Σ are known

$$\theta = \begin{bmatrix} \theta_1 &= \mu \\ \theta_2 &= \Sigma \end{bmatrix} \tag{18}$$

Convert the covariance matrix Σ

$$P(D|\Sigma) = \prod_{k=1}^{n} P(x_k|\Sigma)$$

$$= \prod_{k=1}^{n} \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp(-\frac{1}{2}(x_k - \mu)^T \Sigma^{-1}(x_k - \mu))$$

$$= \frac{1}{((2\pi)^d |\Sigma|)^{n/2}} \exp(-\frac{1}{2} \sum_{n=1}^{k=1} (x_k - \mu)^T \Sigma^{-1}(x_k - \mu))$$
(19)

The property of matrix trace

- scalar $b^T B b = trace(b^T B b) = trace(B b b^T)$
- trace(A + B) = trace(A) + trace(B)
- trace(C(A + B)) = trace(CA) + trace(CB)
- trace(A) is the sum of A's eigenvalues

$$\sum_{n}^{k=1} (x_{k} - \mu)^{T} \Sigma^{-1}(x_{k} - \mu) = \sum_{n}^{k=1} trace((x_{k} - \mu)^{T} \Sigma^{-1}(x_{k} - \mu))$$

$$= \sum_{n}^{k=1} trace(\Sigma^{-1}(x_{k} - \mu)(x_{k} - \mu)^{T})$$

$$= trace(\Sigma^{-1} \sum_{n}^{k=1} (x_{k} - \mu)(x_{k} - \mu)^{T})$$
(20)

Assume

$$A = \frac{1}{n} \sum_{k=1}^{n} (x_k - \mu)(x_k - \mu)^T$$
 (21)

and A is fixed.

Then

$$\sum_{n=1}^{k=1} (x_k - \mu)^T \Sigma^{-1}(x_k - \mu) = n \ trace(\Sigma^{-1}A)$$
 (22)

Therefore

$$P(D|\Sigma) = \frac{1}{((2\pi)^d|\Sigma|)^{n/2}} \exp(-\frac{n}{2} trace(\Sigma^{-1}A))$$
(23)

Assume

$$B = \Sigma^{-1}A \tag{24}$$

and B's eigenvalues are $\lambda_1, \lambda_2, \dots, \lambda_d$

The property of matrix determinant

- det(AB) = det(A)det(B)
- $det(A^{-1}) = det(A)^{-1}$
- det(A) is the product of A's eigenvalues

Therefore

$$P(D|\Sigma) = \frac{1}{((2\pi)^{d}|\Sigma|)^{n/2}} \exp(-\frac{n}{2}trace(\Sigma^{-1}A))$$

$$= \frac{1}{(2\pi)^{dn/2}} |\Sigma|^{-n/2} \exp(-\frac{n}{2}trace(B))$$

$$= \frac{1}{(2\pi)^{dn/2}} (\frac{|B|}{|A|})^{n/2} \exp(-\frac{n}{2}trace(B))$$

$$= \frac{1}{(2\pi)^{dn/2}} |A|^{-n/2} (\prod_{i=1}^{d} \lambda_i)^{n/2} \exp(-\frac{n}{2} \sum_{i=1}^{d} \lambda_i)$$
(25)

$$\log(P(D|\Sigma)) = -\frac{dn}{2}\log(2\pi) - \frac{n}{2}\log(|A|) + \frac{n}{2}\sum_{i=1}^{d}\log(\lambda_i) - \frac{n}{2}\sum_{i=1}^{d}\lambda_i$$
 (26)

$$\frac{\partial(\log(P(x|\Sigma)))}{\partial\lambda_i} = \frac{n}{2\lambda_i} - \frac{n}{2} = 0 \Rightarrow \lambda_i = 1$$
 (27)

Therefore $B \sim I$, and $\Sigma^{-1}A = I \Rightarrow \hat{\Sigma} = A = \frac{1}{n} \sum_{k=1}^{n} (x_k - \mu)(x_k - \mu)^T$.

3.2 Bayesian Estimation (BE)

Steps:

- The parameters are assumed to be random variables with some known priori distribution.
- Bayesian approach aims at estimating the posterior density $P(\theta|D)$
- The MAPE(Maximum A Posteriori Estimate) of θ is the value of θ that maximizes the posterior density $P(\theta|D)$.

Method:

- Estimate P(x|D) from sample data, and assume it has a known parametric form. So $P(x|\theta)$ is completely known, but θ is random variable and has its own PDF.
- $P(x|D) = \int P(x,\theta|D)d\theta = \int P(x|\theta)P(\theta|D)d\theta$
- Posterior $P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$, where $P(D|\theta) = \prod_{k=1}^{n} P(x_k|\theta)$
- Since P(D) is constant, therefore $\hat{\theta} = \arg \max_{\theta} \{P(D|\theta)P(\theta)\}\$

3.2.1 E.g. Univariate Gaussian

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3.2.2 E.g. Multivariate Gaussian

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4 Principle Component Analysis (PCA)