Probabilistic classification

Machine Learning

Hamid R Rabiee – Zahra Dehghanian Spring 2025



Topics

- Probabilistic approach
 - Bayes decision theory
 - Generative models
 - Gaussian Bayes classifier
 - Naïve Bayes



Classification problem: probabilistic view

- Given: Training set
 - labeled set of N input-output pairs $D = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$
 - ▶ $y \in \{1, ..., K\}$
- Goal: Given an input x, assign it to one of K classes
- Examples:
 - Spam filter
 - Handwritten digit recognition
 - **...**



Definitions

- Posterior probability: $p(C_k|x)$
- Likelihood or class conditional probability: $p(x|\mathcal{C}_k)$
- Prior probability: $p(C_k)$

$$p(x)$$
: pdf of feature vector x ($p(x) = \sum_{k=1}^{K} p(x|\mathcal{C}_k)p(\mathcal{C}_k)$)

 $p(x|\mathcal{C}_k)$: pdf of feature vector x for samples of class \mathcal{C}_k

 $p(\mathcal{C}_k)$: probability of the label be \mathcal{C}_k



Bayes decision rule

K=2

If
$$P(C_1|x) > P(C_2|x)$$
 decide C_1 otherwise decide C_2

$$p(error|\mathbf{x}) = \begin{cases} p(C_2|\mathbf{x}) & \text{if we decide } C_1 \\ P(C_1|\mathbf{x}) & \text{if we decide } C_2 \end{cases}$$

If we use Bayes decision rule:

$$P(error|\mathbf{x}) = \min\{P(\mathcal{C}_1|\mathbf{x}), P(\mathcal{C}_2|\mathbf{x})\}\$$

Using Bayes rule, for each x, P(error|x) is as small as possible and thus this rule minimizes the probability of error



Optimal classifier

 The optimal decision is the one that minimizes the expected number of mistakes

We show that Bayes classifier is an optimal classifier



Bayes decision rule Minimizing misclassification rate

▶ Decision regions: $\mathcal{R}_k = \{x | \alpha(x) = k\}$

K = 2

All points in \mathcal{R}_k are assigned to class \mathcal{C}_k

$$p(error) = E_{x,y}[I(\alpha(x) \neq y)]$$

$$= p(x \in \mathcal{R}_1, \mathcal{C}_2) + p(x \in \mathcal{R}_2, \mathcal{C}_1)$$

$$= \int_{\mathcal{R}_1} p(x, \mathcal{C}_2) dx + \int_{\mathcal{R}_2} p(x, \mathcal{C}_1) dx$$

$$= \int_{\mathcal{R}_1} p(\mathcal{C}_2|x)p(x) dx + \int_{\mathcal{R}_2} p(\mathcal{C}_1|x)p(x) dx$$

Choose class with highest $p(C_k|\mathbf{x})$ as $\alpha(\mathbf{x})$



Bayes minimum error

Bayes minimum error classifier:

$$\min_{\alpha(.)} E_{x,y}[I(\alpha(x) \neq y)]$$
 Zero-one loss

 If we know the probabilities in advance then the above optimization problem will be solved easily.

•
$$\alpha(\mathbf{x}) = \underset{\mathbf{y}}{\operatorname{argmax}} p(\mathbf{y}|\mathbf{x})$$

• In practice, we can estimate p(y|x) based on a set of training samples $\mathcal D$



Bayes theorem

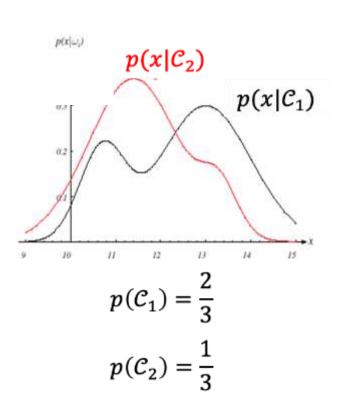
- Posterior
 Posterior $p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}$
- Posterior probability: $p(C_k|x)$
- Likelihood or class conditional probability: $p(x|\mathcal{C}_k)$
- Prior probability: $p(C_k)$

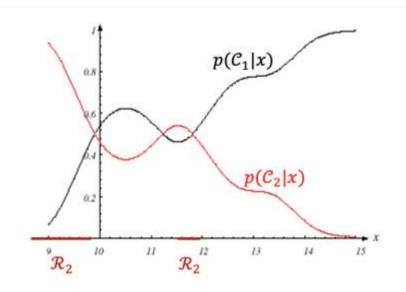
p(x): pdf of feature vector x ($p(x) = \sum_{k=1}^{K} p(x|\mathcal{C}_k)p(\mathcal{C}_k)$) $p(x|\mathcal{C}_k)$: pdf of feature vector x for samples of class \mathcal{C}_k $p(\mathcal{C}_k)$: probability of the label be \mathcal{C}_k



Bayes decision rule: example

• Bayes decision: Choose the class with highest $p(C_k|x)$





$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}$$
$$p(\mathbf{x}) = p(C_1)p(\mathbf{x}|C_1) + p(C_2)p(\mathbf{x}|C_2)$$



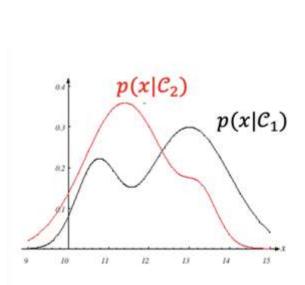
Bayesian decision rule

- If $P(C_1|x) > P(C_2|x)$ decide C_1 otherwise decide C_2 Equivalent
- If $\frac{p(x|\mathcal{C}_1)P(\mathcal{C}_1)}{p(x)} > \frac{p(x|\mathcal{C}_2)P(\mathcal{C}_2)}{p(x)}$ decide \mathcal{C}_1 otherwise decide \mathcal{C}_2 Equivalent
- If $p(x|C_1)P(C_1) > p(x|C_2)P(C_2)$ decide C_1 otherwise decide C_2



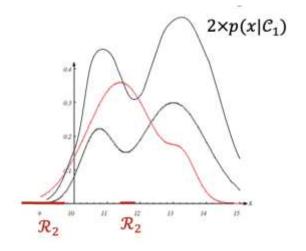
Bayes decision rule: example

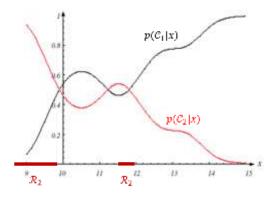
• Bayes decision: Choose the class with highest $p(C_k|x)$



$$p(\mathcal{C}_1) = \frac{2}{3}$$

$$p(\mathcal{C}_2) = \frac{1}{3}$$





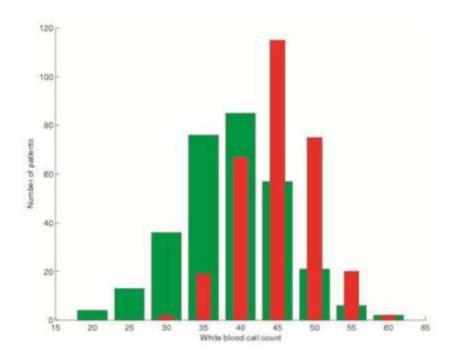


Bayes Classier

- Simple Bayes classifier: estimate posterior probability of each class
- What should the decision criterion be?
 - Choose class with highest $p(C_k|x)$
- The optimal decision is the one that minimizes the expected number of mistakes



white blood cell count



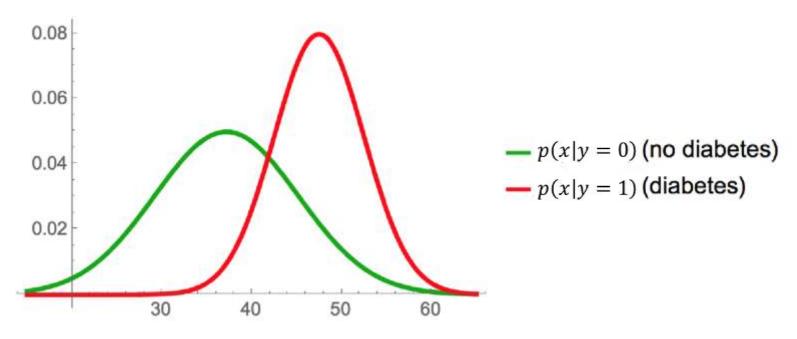
This example has been adopted from Sanja Fidler's slides, University of Toronto, CSC411



- Doctor has a prior p(y = 1) = 0.2
 - Prior: In the absence of any observation, what do I know about the probability of the classes?
- A patient comes in with white blood cell count x
- Does the patient have diabetes p(y = 1|x)?
 - given a new observation, we still need to compute the posterior



$$p(x = 40|y = 0)P(y = 0) > p(x = 40|y = 1)P(y = 1)$$



This example has been adopted from Sanja Fidler's slides, University of Toronto, CSC411



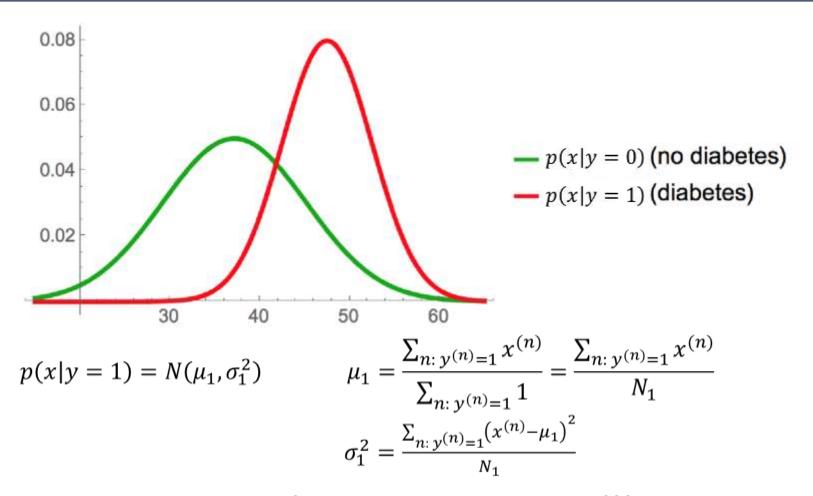
Estimate probability densities from data

- If we assume Gaussian distributions for p(x|y=0) and p(x|y=1)
- Recall that for samples $\{x^{(1)}, ..., x^{(N)}\}$, if we assume a Gaussian distribution, the MLE estimates will be

$$\mu = \frac{1}{N} \sum_{n=1}^{N} x^{(n)}$$

$$\sigma^{2} = \frac{1}{N} \sum_{n=1}^{N} (x^{(n)} - \mu)^{2}$$

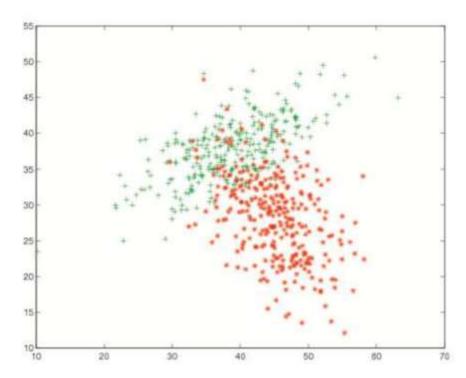




This example has been adopted from Sanja Fidler's slides, University of Toronto, CSC411



Add a second observation: Plasma glucose value



This example has been adopted from Sanja Fidler's slides, University of Toronto, CSC411



Naïve Bayes classifier

- Generative methods
 - High number of parameters
- Assumption: Conditional independence

$$p(\mathbf{x}|C_k) = p(x_1|C_k) \times p(x_2|C_k) \times \dots \times p(x_d|C_k)$$



Naïve Bayes classifier

• In the decision phase, it finds the label of x according to:

$$\underset{k=1,\dots,K}{\operatorname{argmax}} p(C_k | \mathbf{x})$$

$$\underset{k=1,\dots,K}{\operatorname{argmax}} p(C_k) \prod_{i=1}^{n} p(x_i | C_k)$$

$$p(\mathbf{x}|C_k) = p(x_1|C_k) \times p(x_2|C_k) \times \dots \times p(x_d|C_k)$$
$$p(C_k|\mathbf{x}) \propto p(C_k) \prod_{i=1}^n p(x_i|C_k)$$



Naïve Bayes: discrete example

•
$$p(h) = 0.3$$

•
$$p(d|h) = \frac{1}{3}$$

• $p(s|h) = \frac{2}{3}$

•
$$p(s|h) = \frac{2}{3}$$

•
$$p(d|\bar{h}) = \frac{2}{7}$$

•
$$p(s|\bar{h}) = \frac{2}{7}$$

$$H = Yes \equiv h$$

 $H = No \equiv \bar{h}$

Diabetes (D)	Smoke (S)	Heart Disease (H)
Y	N	Y
Y	N	N
N	Y	N
N	Y	N
N	N	N
N	Y	Y
N	N	N
N	Y	Y
N	N	N
Y	N	N



Naïve Bayes: discrete example

•
$$p(h) = 0.3$$

•
$$p(d|h) = \frac{1}{3}$$

•
$$p(s|h) = \frac{2}{3}$$

•
$$p(d|\bar{h}) = \frac{2}{7}$$

•
$$p(s|\bar{h}) = \frac{2}{7}$$

$$H = Yes \equiv h$$

 $H = No \equiv \bar{h}$

Diabetes (D)	Smoke (S)	Heart Disease (H)
Y	N	Y
Y	N	N
N	Y	N
N	Y	N
N	N	N
N	Y	Y
N	N	N
N	Y	Y
N	N	N
Y	N	N

- Decision on $x = [d, \bar{s}]$ (a person that has diabetes but does not smoke):
 - $p(h|\mathbf{x}) \propto p(h)p(d|h)p(\bar{s}|h) = 1/14$
 - $p(\bar{h}|\mathbf{x}) \propto p(\bar{h})p(d|\bar{h})p(\bar{s}|\bar{h}) = 1/6$
 - Thus decide H = No



Naïve Bayes classifier

- Finds d univariate distributions $p(x_1|C_k), \cdots, p(x_d|C_k)$ instead of finding one multi-variate distribution $p(x|C_k)$
 - Example 1: For Gaussian class-conditional density $p(x|C_k)$, it finds d+d (mean and sigma parameters on different dimensions) instead of $d+\frac{d(d+1)}{2}$ parameters
 - Example 2: For Bernoulli class-conditional density $p(x|C_k)$, it finds d (mean parameters on different dimensions) instead of 2^d-1 parameters
- It first estimates the class conditional densities $p(x_1|C_k), \cdots, p(x_d|C_k)$ and the prior probability $p(C_k)$ for each class $(k=1,\ldots,K)$ based on the training set.



Multivariate Gaussian

• For samples $\{x^{(1)}, ..., x^{(N)}\}$, if we assume a multivariate Gaussian distribution, the MLE estimates will be:

$$\boldsymbol{\mu} = \frac{\sum_{n=1}^{N} \boldsymbol{x}^{(n)}}{N}$$

$$\Sigma = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}^{(n)} - \boldsymbol{\mu}) (\mathbf{x}^{(n)} - \boldsymbol{\mu})^{T}$$



Multivariate Gaussian

• Multivariate Gaussian distributions for
$$p(x|\mathcal{C}_k)$$
:
$$p(x|y=k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\{-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k)\}$$

$$k = 1,2$$

• Prior distribution p(y):

•
$$p(y = 1) = \pi$$
, $p(y = 0) = 1 - \pi$



Multivariate Gaussian

Maximum likelihood estimation (D

$$= \{ (x^{(n)}, y^{(n)}) \}_{n=1}^{N}):$$

•
$$\pi = \frac{N_1}{N}$$

•
$$\mu_1 = \frac{\sum_{n=1}^{N} y^{(n)} x^{(n)}}{N_1}$$
, $\mu_2 = \frac{\sum_{n=1}^{N} (1 - y^{(n)}) x^{(n)}}{N_2}$

•
$$\Sigma_1 = \frac{1}{N_1} \sum_{n=1}^{N} y^{(n)} (x^{(n)} - \mu) (x^{(n)} - \mu)^T$$

•
$$\Sigma_2 = \frac{1}{N_2} \sum_{n=1}^{N} (1 - y^{(n)}) (x^{(n)} - \mu) (x^{(n)} - \mu)^T$$

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

$$N_1 = \sum_{n=1}^N y^{(n)}$$

$$N_2 = N - N_1$$



Decision boundary for Gaussian Bayes classifier

$$p(\mathcal{C}_1|\mathbf{x}) = p(\mathcal{C}_2|\mathbf{x})$$

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}$$

$$\ln p(\mathcal{C}_1|\mathbf{x}) = \ln p(\mathcal{C}_2|\mathbf{x})$$

$$\ln p(\mathbf{x}|\mathcal{C}_1) + \ln p(\mathcal{C}_1) - \ln p(\mathbf{x})$$

= $\ln p(\mathbf{x}|\mathcal{C}_2) + \ln p(\mathcal{C}_2) - \ln p(\mathbf{x})$



Decision boundary for Gaussian Bayes classifier

•
$$p(\mathcal{C}_1|\boldsymbol{x}) = p(\mathcal{C}_2|\boldsymbol{x})$$

$$p(\mathcal{C}_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\boldsymbol{x})}$$

$$\ln p(\mathcal{C}_1|\boldsymbol{x}) = \ln p(\mathcal{C}_2|\boldsymbol{x})$$

$$\ln p(\boldsymbol{x}|\mathcal{C}_1) + \ln p(\mathcal{C}_1) - \ln p(\boldsymbol{x})$$

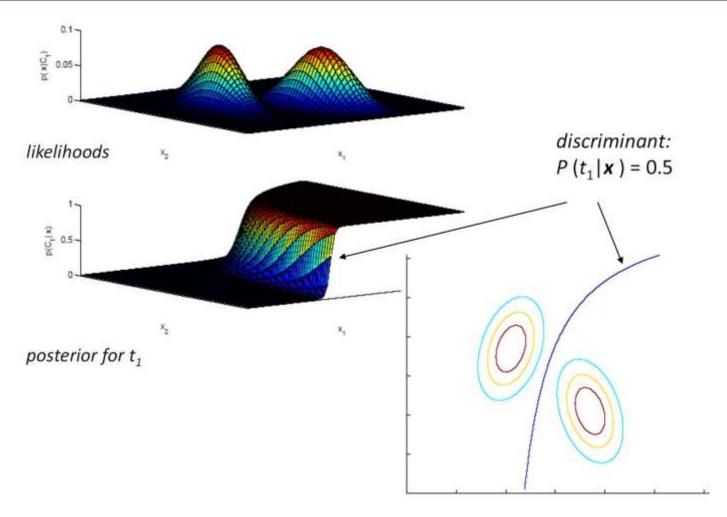
= \ln p(\boldsymbol{x}|\mathcal{C}_2) + \ln p(\mathcal{C}_2) - \ln p(\boldsymbol{x})

$$\ln p(\boldsymbol{x}|\mathcal{C}_1) + \ln p(\mathcal{C}_1) = \ln p(\boldsymbol{x}|\mathcal{C}_2) + \ln p(\mathcal{C}_2)$$

$$\frac{\ln p(\mathbf{x}|\mathcal{C}_k)}{= -\frac{d}{2}\ln 2\pi - \frac{1}{2}\ln |\mathbf{\Sigma}_k| - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^T \mathbf{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)$$



Decision boundary





Shared covariance matrix

m P When classes share a single covariance matrix $m \Sigma = m \Sigma_1 = m \Sigma_2$

$$p(\mathbf{x}|C_k) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)\}$$

$$k = 1,2$$

$$p(C_1) = \pi, \quad p(C_2) = 1 - \pi$$



Likelihood

•
$$\prod_{n=1}^{N} p(\mathbf{x}^{(n)}, y^{(n)}; \pi, \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma})$$

$$= \prod_{n=1}^{N} p(\mathbf{x}^{(n)} | y^{(n)}; \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}) p(y^{(n)}; \pi)$$



Shared covariance matrix

* Maximum likelihood estimation $(D = \{(x^{(i)}, y^{(i)})\}_{i=1}^n)$:

$$\mu_1 = \frac{\sum_{n=1}^{N} y^{(n)} x^{(n)}}{N_1}$$

$$\mu_2 = \frac{\sum_{n=1}^{N} (1 - y^{(n)}) x^{(n)}}{N_2}$$

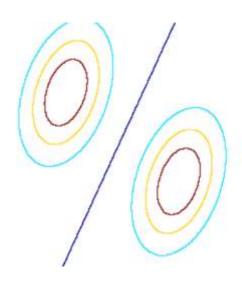
$$\Sigma = \frac{1}{N} \left(\sum_{n \in C_1} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_1) (\mathbf{x}^{(n)} - \boldsymbol{\mu}_1)^T + \sum_{n \in C_2} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_2) (\mathbf{x}^{(n)} - \boldsymbol{\mu}_2)^T \right)$$



Decision boundary when shared covariance matrix

• $\ln p(\mathbf{x}|\mathcal{C}_1) + \ln p(\mathcal{C}_1) = \ln p(\mathbf{x}|\mathcal{C}_2) + \ln p(\mathcal{C}_2)$

$$\ln p(\mathbf{x}|\mathcal{C}_k) = -\frac{d}{2}\ln 2\pi - \frac{1}{2}\ln |\mathbf{\Sigma}| - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^T \mathbf{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_k)$$





Multi-class Bayes decision rule

- Multi-class problem: Probability of error of Bayesian decision rule
 - Simpler to compute the probability of correct decision

$$P(error) = 1 - P(correct)$$

$$P(Correct) = \sum_{i=1}^{K} \int_{\mathcal{R}_i} p(\mathbf{x}, \mathcal{C}_i) d\mathbf{x}$$

$$= \sum_{i=1}^{K} \int_{\mathcal{R}_i} p(\mathcal{C}_i | \mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

 \mathcal{R}_i : the subset of feature space assigned to the class \mathcal{C}_i using the classifier



Bayes minimum error

Bayes minimum error classifier:

$$\min_{\alpha(.)} E_{x,y}[I(\alpha(x) \neq y)]$$
 Zero-one loss

$$\alpha(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{y}} p(\mathbf{y}|\mathbf{x})$$



Minimizing Bayes risk (expected loss)

$$E_{x,y}[L(\alpha(x),y)]$$

$$= \int \sum_{j=1}^{K} L(\alpha(x),C_j)p(x,C_j)dx$$



Minimizing Bayes risk (expected loss)

$$E_{x,y}[L(\alpha(x),y)]$$

$$= \int \sum_{j=1}^{K} L(\alpha(x), C_j) p(x, C_j) dx$$

$$= \int p(x) \sum_{j=1}^{K} L(\alpha(x), C_j) p(C_j|x) dx$$

for each x minimize it that is called conditional risk



Minimizing Bayes risk (expected loss)

$$E_{x,y}[L(\alpha(x), y)]$$

$$= \int \sum_{j=1}^{K} L(\alpha(x), C_j) p(x, C_j) dx$$

$$= \int p(x) \sum_{j=1}^{K} L(\alpha(x), C_j) p(C_j | x) dx$$

for each x minimize it that is called conditional risk

▶ Bayes minimum loss (risk) decision rule: $\hat{\alpha}(x)$

$$\hat{\alpha}(\mathbf{x}) = \underset{i=1,...,K}{\operatorname{argmin}} \sum_{j=1}^{K} \underline{L_{ij}} p(\mathcal{C}_{j}|\mathbf{x})$$

The loss of assigning a sample to C_i where the correct class is C_j



Minimizing expected loss: special case (loss = misclassification rate)

- Problem definition for this special case:
 - If action $\alpha(x) = i$ is taken and the true category is C_j , then the decision is correct if i = j and otherwise it is incorrect.
 - Zero-one loss function:

$$L_{ij} = 1 - \delta_{ij} = \begin{cases} 0 & i = j \\ 1 & o.w. \end{cases}$$

$$\hat{\alpha}(\mathbf{x}) = \underset{i=1,...,K}{\operatorname{argmin}} \sum_{j=1}^{K} L_{ij} p(\mathcal{C}_j | \mathbf{x})$$



Minimizing expected loss: special case (loss = misclassification rate)

- Problem definition for this special case:
 - If action $\alpha(x) = i$ is taken and the true category is C_j , then the decision is correct if i = j and otherwise it is incorrect.
 - Zero-one loss function:

$$L_{ij} = 1 - \delta_{ij} = \begin{cases} 0 & i = j \\ 1 & o. w. \end{cases}$$

$$\hat{\alpha}(\mathbf{x}) = \underset{i=1,...,K}{\operatorname{argmin}} \sum_{j=1}^{K} L_{ij} p(\mathcal{C}_j | \mathbf{x})$$

= argmin_{i=1,...,K}
$$0 \times p(C_i|\mathbf{x}) + \sum_{j \neq i} p(C_j|\mathbf{x})$$

$$= \underset{i=1,\dots,K}{\operatorname{argmin}} 1 - p(\mathcal{C}_i|\boldsymbol{x}) = \underset{i=1,\dots,K}{\operatorname{argmax}} p(\mathcal{C}_i|\boldsymbol{x})$$



Probabilistic classifiers

- How can we find the probabilities required in the Bayes decision rule?
- Probabilistic classification approaches can be divided in two main categories:
 - Generative
 - Estimate pdf $p(x, C_k)$ for each class C_k and then use it to find $p(C_k|x)$
 - \Box or alternatively estimate both pdf $p(x|\mathcal{C}_k)$ and $p(\mathcal{C}_k)$ to find $p(\mathcal{C}_k|x)$
 - Discriminative
 - ▶ Directly estimate $p(C_k|x)$ for each class C_k



Generative approach

- Inference stage
 - Determine class conditional densities $p(x|\mathcal{C}_k)$ and priors $p(\mathcal{C}_k)$
 - Use the Bayes theorem to find $p(C_k|x)$

- Decision stage: After learning the model (inference stage), make optimal class assignment for new input
 - if $p(C_i|x) > p(C_j|x) \quad \forall j \neq i$ then decide C_i



Probabilistic discriminant functions

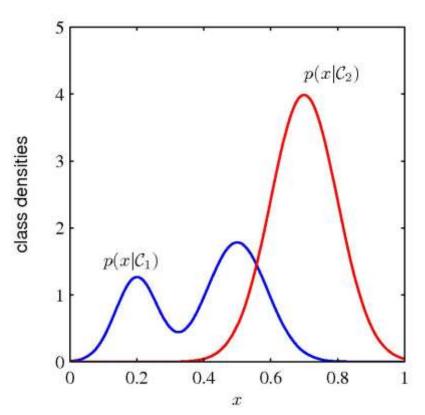
- Discriminant functions: A popular way of representing a classifier
 - A discriminant function $f_i(x)$ for each class C_i (i = 1, ..., K):
 - x is assigned to class C_i if:

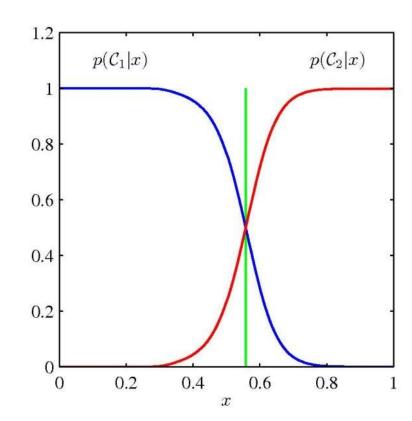
$$f_i(\mathbf{x}) > f_j(\mathbf{x}) \ \forall j \neq i$$

- Representing Bayesian classifier using discriminant functions:
 - Classifier minimizing error rate: $f_i(\mathbf{x}) = P(C_i|\mathbf{x})$
 - Classifier minimizing risk: $f_i(\mathbf{x}) = -\sum_{j=1}^K L_{ij} p(\mathcal{C}_j | \mathbf{x})$



Discriminative vs. generative approach

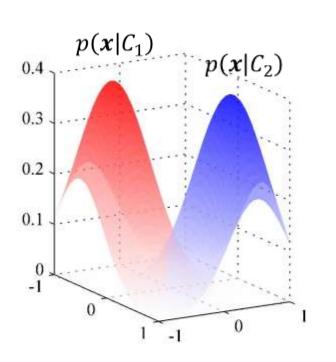


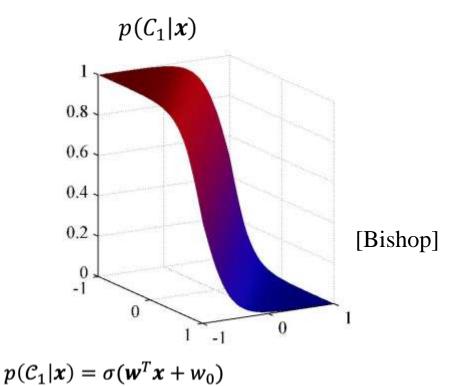


[Bishop]



Class conditional densities vs. posterior





$$\sigma(z) = \frac{1}{1 + \exp(z)}$$

$$\mathbf{w} = \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

$$w_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_2 + \ln \frac{p(C_1)}{p(C_2)}$$



Feed back

? https://forms.gle/vKRbyVVsWRKcZuqr8



Resources

- C. Bishop, "Pattern Recognition and Machine Learning", Chapter 4.2-4.3.
- Course CE-717, Dr. M.Soleymani

