Probabilistic Generative Models

Classification so far

First solve the inference problem of determining the posterior class probabilities $p(\mathcal{C}_k|\mathbf{x})$, and then subsequently use decision theory to assign each new $\mathbf{x}$ to one of the classes. Approaches that model the posterior probabilities directly are called *discriminative models*.

Find a function $f(\mathbf{x})$, called a discriminant function, which maps each input $\mathbf{x}$ directly onto a class label. For instance, in the case of two-class problems, $f(\cdot)$ might be binary valued and such that $f = 0$ represents class $\mathcal{C}_1$ and $f = 1$ represents class $\mathcal{C}_2$. In this case, probabilities play no role.

Generative classifiers

First solve the inference problem of determining the class-conditional densities $p(\mathbf{x}|\mathcal{C}_k)$ for each class $\mathcal{C}_k$ individually. Also separately infer the prior class probabilities $p(\mathcal{C}_k)$. Then use Bayes' theorem in the form

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

Equivalently, we can model the joint distribution $p(\mathbf{x}, C_k)$ directly and then normalize to obtain the posterior probabilities

Approaches that explicitly or implicitly model the distribution of inputs as well as outputs are known as ***generative models***

Probabilistic Generative Models

Approaches that explicitly or implicitly model the distribution of inputs as well as outputs are known as **generative models**, because by sampling from them it is possible to generate synthetic data points in the input space.
Approaches that model the posterior probabilities directly are called **discriminative models**

$$
\begin{aligned}
p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\
&= \frac{1}{1+\exp(-a)} = \sigma(a)
\end{aligned}
$$

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

$$
\begin{aligned}
p(\mathcal{C}_k|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} \\
&= \frac{\exp(a_k)}{\sum_j \exp(a_j)}
\end{aligned}
$$

$$a_k = \ln p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k).$$

Probabilistic Generative Models

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

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu}_k) \right\}.$$

Probabilistic Generative Models

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$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$$

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ w_0 &= -\frac{1}{2}\boldsymbol{\mu}_1^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}. \end{aligned}$$

Probabilistic Generative Models

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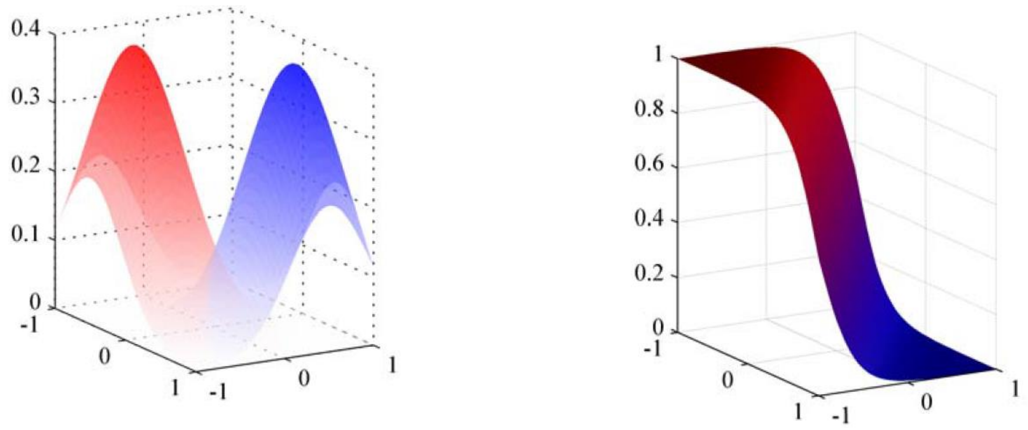

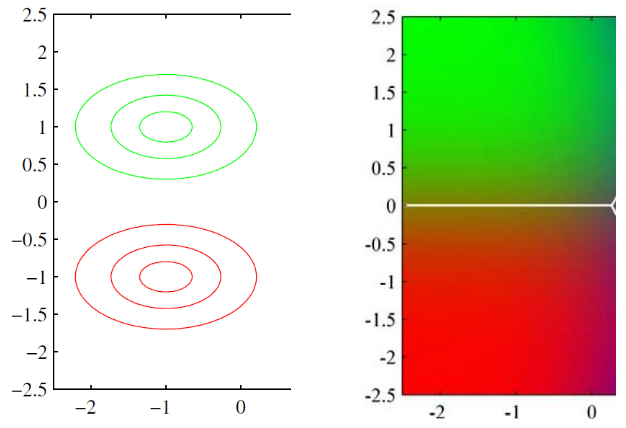

Probabilistic Generative Models

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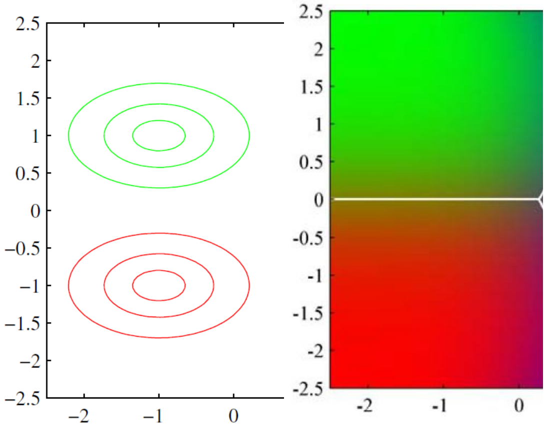

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$$

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$$\begin{aligned} p(\mathcal{C}_k|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} \\ &= \frac{\exp(a_k)}{\sum_j \exp(a_j)} \end{aligned}$$

$$a_k = \ln p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k).$$

$$a_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

$$\begin{aligned} \mathbf{w}_k &= \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k \\ w_{k0} &= -\frac{1}{2}\boldsymbol{\mu}_k^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \ln p(\mathcal{C}_k). \end{aligned}$$

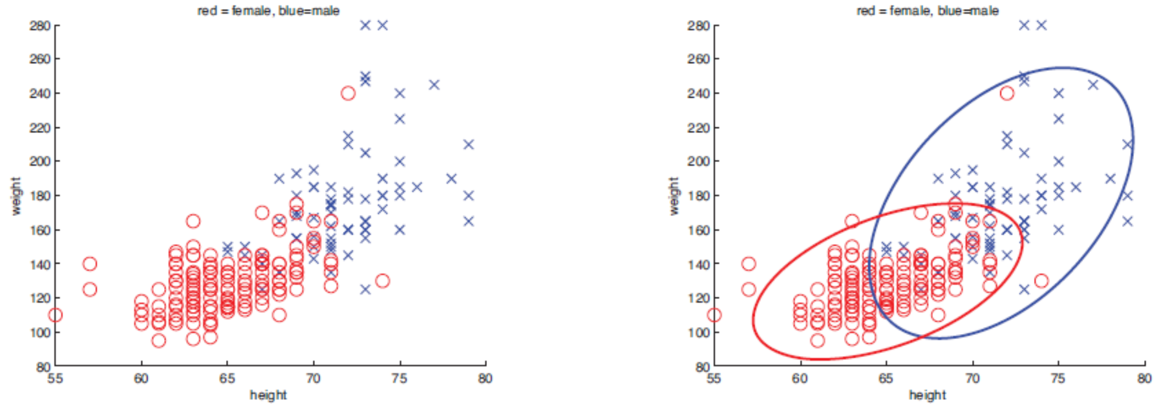
Probabilistic Generative Models

model the **class-conditional densities *p*(x/*C*$_k$)**, as well as the **class priors *p*(*C*$_k$)**

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

class-conditional densities *p*(x/*C*)

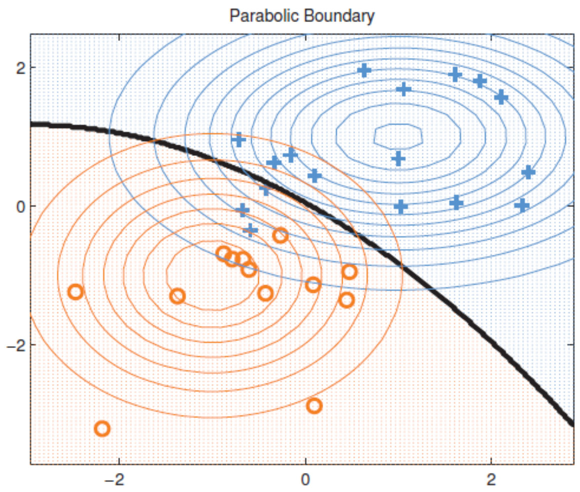
$$p(\mathbf{x}|y = c, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$



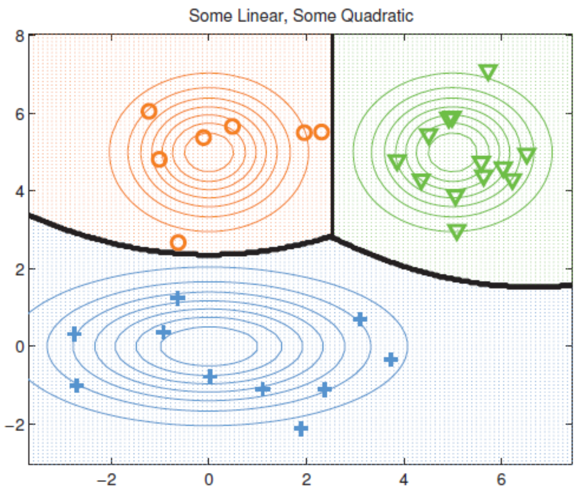
(a) (b)

Quadratic discriminant analysis

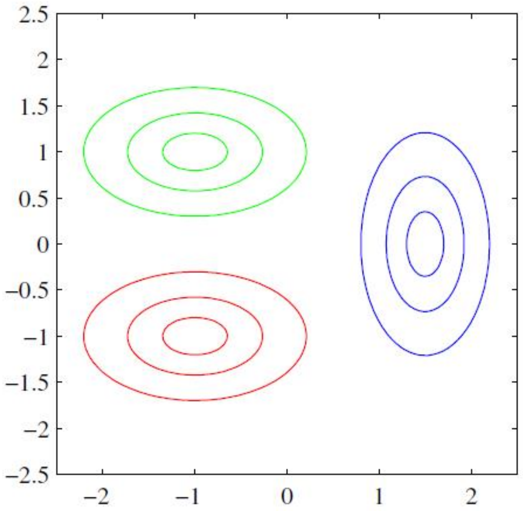
$$p(y=c|\mathbf{x},\boldsymbol{\theta}) = \frac{\pi_c|2\pi\boldsymbol{\Sigma}_c|^{-\frac{1}{2}}\exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_c)^T\boldsymbol{\Sigma}_c^{-1}(\mathbf{x}-\boldsymbol{\mu}_c)\right]}{\sum_{c'}\pi_{c'}|2\pi\boldsymbol{\Sigma}_{c'}|^{-\frac{1}{2}}\exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_{c'})^T\boldsymbol{\Sigma}_{c'}^{-1}(\mathbf{x}-\boldsymbol{\mu}_{c'})\right]}$$

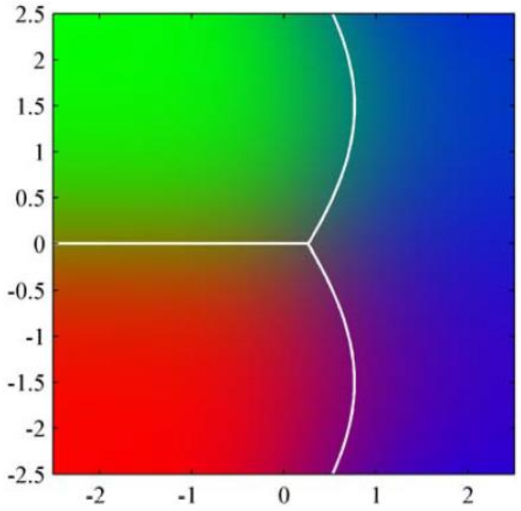


(a)



(b)





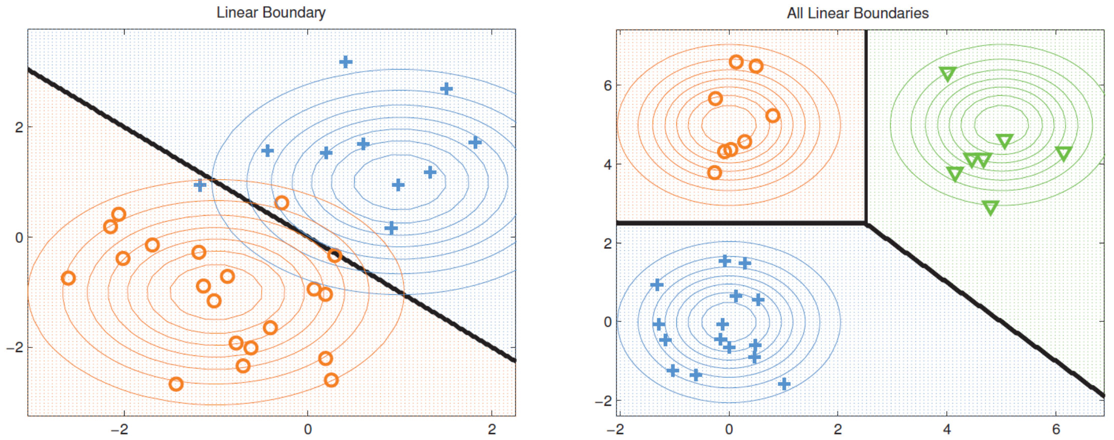
Linear Discriminant Analysis

- covariance matrices are **tied** or **shared** across classes, **Σ***c* = **Σ**.

$$
\begin{aligned}
p(y=c|\mathbf{x},\boldsymbol{\theta}) &\propto \pi_c \exp\left[\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right] \\
&= \exp\left[\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c + \log\pi_c\right]\exp[-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}]
\end{aligned}
$$

$$
p(y=c|\mathbf{x},\boldsymbol{\theta}) = \frac{e^{\boldsymbol{\beta}_c^T\mathbf{x}+\gamma_c}}{\sum_{c'} e^{\boldsymbol{\beta}_{c'}^T\mathbf{x}+\gamma_{c'}}}
$$

$$
\begin{aligned}
\gamma_c &= -\frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c + \log\pi_c \\
\boldsymbol{\beta}_c &= \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c
\end{aligned}
$$



Generative Models: Parameter estimation

- Models joint probability of observing input and output

$$p(\mathbf{x}_n, \mathcal{C}_1) = p(\mathcal{C}_1)p(\mathbf{x}_n|\mathcal{C}_1) = \pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}).$$

$$p(\mathbf{x}_n, \mathcal{C}_2) = p(\mathcal{C}_2)p(\mathbf{x}_n|\mathcal{C}_2) = (1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}).$$

$$p(\mathbf{t}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \left[\pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})\right]^{t_n} \left[(1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})\right]^{1-t_n}$$

Generative Models : Parameter estimation

- Models joint probability of observing input and output

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \left[\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbb{I}(y_i = c)\log \pi_c\right] + \sum_{c=1}^{C}\left[\sum_{i:y_i=c}\log \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)\right]$$

Use **Maximum Likelihood Estimation (MLE)** to estimate parameters

Generative Models : Parameter estimation

- Models joint probability of observing input and output

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \left[\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbb{I}(y_i = c)\log \pi_c\right] + \sum_{c=1}^{C}\left[\sum_{i:y_i=c}\log \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)\right]$$

$$\hat{\pi}_c = \frac{N_c}{N}, \qquad \hat{\boldsymbol{\mu}}_c = \frac{1}{N_c}\sum_{i:y_i=c}\mathbf{x}_i, \quad \hat{\boldsymbol{\Sigma}}_c = \frac{1}{N_c}\sum_{i:y_i=c}(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_c)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_c)^T$$

- MLE can badly overfit in high dimensions.
- Use a diagonal covariance matrix for each class, which assumes the features are conditionally independent; this is equivalent to using a **naive Bayes classifier**
- Other approaches : Use **MAP** and **Bayesian approaches**

Naïve Bayes Classifier

- Features are discrete

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

- class-conditional density p(x|y)
  - Number of parameters ?

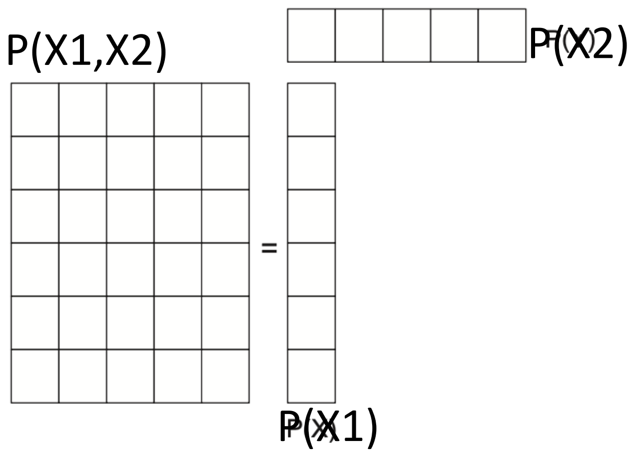
Naïve Bayes Classifier

- Features are discrete

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

- "naive" since we do not expect the features to be independent, but results in classifiers that work well
    - model is quite simple and hence it is relatively immune to overfitting, as a lower number of parameters need to be estimated due to independence assumption.
- Class-conditional density p(x|y)

$$p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} p(x_j|y=c,\boldsymbol{\theta}_{jc})$$



Naïve Bayes Classifier

- Features are conditionally independent given the class label.

$$p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} p(x_j|y=c,\boldsymbol{\theta}_{jc})$$

- class-conditional density p(x|y)
  - In the case of real-valued features, we can use the Gaussian distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \mathcal{N}(x_j|\mu_{jc},\sigma_{jc}^2)$, where μ_{jc} is the mean of feature j in objects of class c, and σ_{jc}^2 is its variance.
  - In the case of binary features, $x_j \in \{0,1\}$, we can use the Bernoulli distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \mathrm{Ber}(x_j|\mu_{jc})$, where μ_{jc} is the probability that feature j occurs in class c.
  - In the case of categorical features, $x_j \in \{1,\ldots,K\}$, we can model use the multinoulli distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \mathrm{Cat}(x_j|\boldsymbol{\mu}_{jc})$, where $\boldsymbol{\mu}_{jc}$ is a histogram over the K possible values for x_j in class c.

Training NBC : ML Estimation

$$p(\mathbf{x}_i, y_i|\boldsymbol{\theta}) = p(y_i|\boldsymbol{\pi}) \prod_j p(x_{ij}|\boldsymbol{\theta}_j) = \prod_c \pi_c^{\mathbb{I}(y_i=c)} \prod_j \prod_c p(x_{ij}|\boldsymbol{\theta}_{jc})^{\mathbb{I}(y_i=c)}$$

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{j=1}^{D} \sum_{c=1}^{C} \sum_{i:y_i=c} \log p(x_{ij}|\boldsymbol{\theta}_{jc})$$

Bernoulli class condiitonal likelihood

$$\hat{\pi}_c = \frac{N_c}{N} \qquad \hat{\theta}_{jc} = \frac{N_{jc}}{N_c}$$

The method is easily generalized to handle features of mixed type.

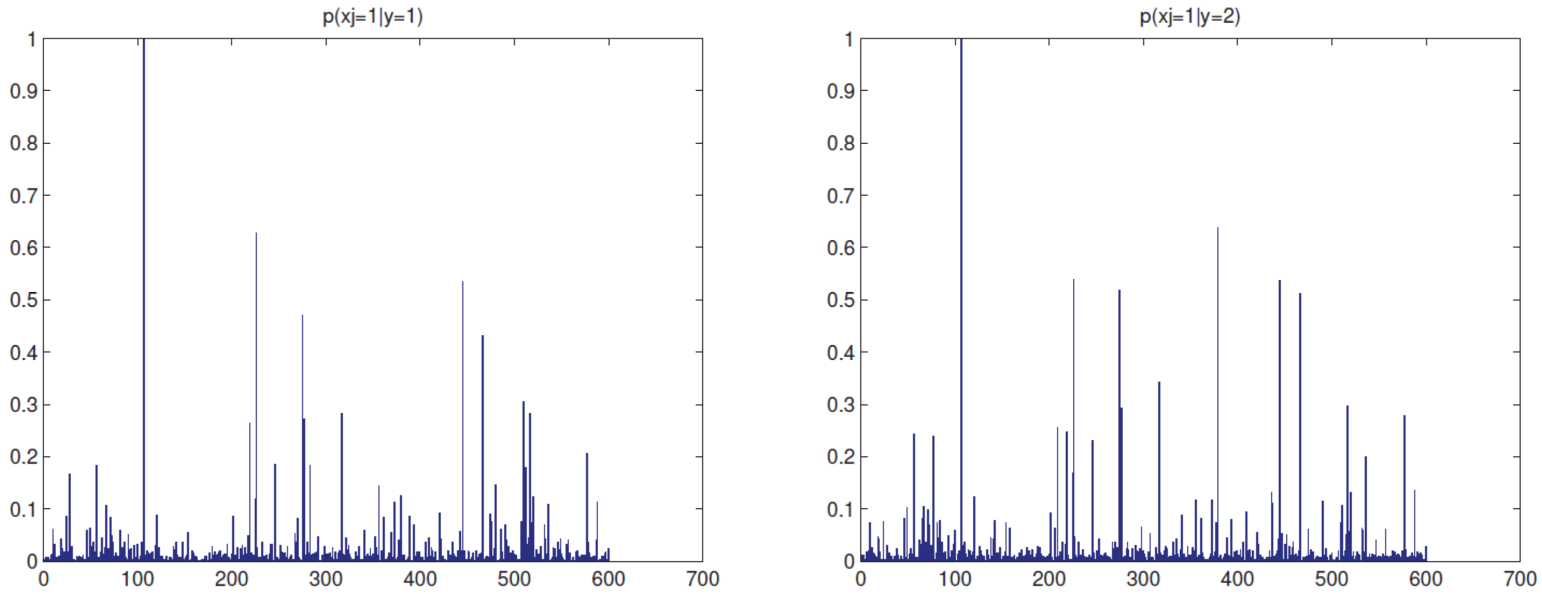
NBC : Algorithm

Algorithm 3.1: Fitting a naive Bayes classifier to binary features

$N_c = 0, N_{jc} = 0;$
for $i = 1 : N$ **do**
    $c = y_i$ // Class label of i'th example;
    $N_c := N_c + 1$;
    for $j = 1 : D$ **do**
        if $x_{ij} = 1$ **then**
            $N_{jc} := N_{jc} + 1$

$\hat{\pi}_c = \frac{N_c}{N}$, $\hat{\theta}_{jc} = \frac{N_{jc}}{N}$

$O(ND)$ time.



(a) (b)

Spam Classification example

HAM examples	**SPAM examples**
• d1: {good} • d2: {very good} P(y=ham)= 2/5	• d3: {bad} • d4: {very bad} • d5: {very bad very bad} p(y=spam)= 3/5

- Test data: d6: {good bad very bad} - **SPAM OR HAM??**
- Vocabulary : V={good, bad, very}
- Use Naive Bayes classifier:
- P(ham | d6)= $\prod$ P(word | y=ham) P(y=ham)

  = P(good | ham) * P(bad | ham) * P(very | ham)

Word frequencies wrt class	P(good | y)	P(bad | y)	P(very | y)
Class 0: y = spam	0/3	3/3	2/3
Class 1: y = ham	2/2	0/2	1/2

- Estimate parameters using ML:
- P(ham | d6)= P(good | ham) * P(bad | ham) * P(very | ham)* P(ham)
- P(spam | d6)= P(good | spam) * P(bad | spam) * P(very | spam)* P(spam)

- What is the problem with this ?

Word frequencies wrt class	P(good | y)	P(bad | y)	P(very | y)
Class 0: y = spam	0/3	3/3	2/3
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- Estimate parameters using ML:
- P(ham | d6)= P(good | ham) * P(bad | ham) * P(very | ham)* P(ham)
- P(spam | d6)= P(good | spam) * P(bad | spam) * P(very | spam)* P(spam)

- What is the problem with this ?

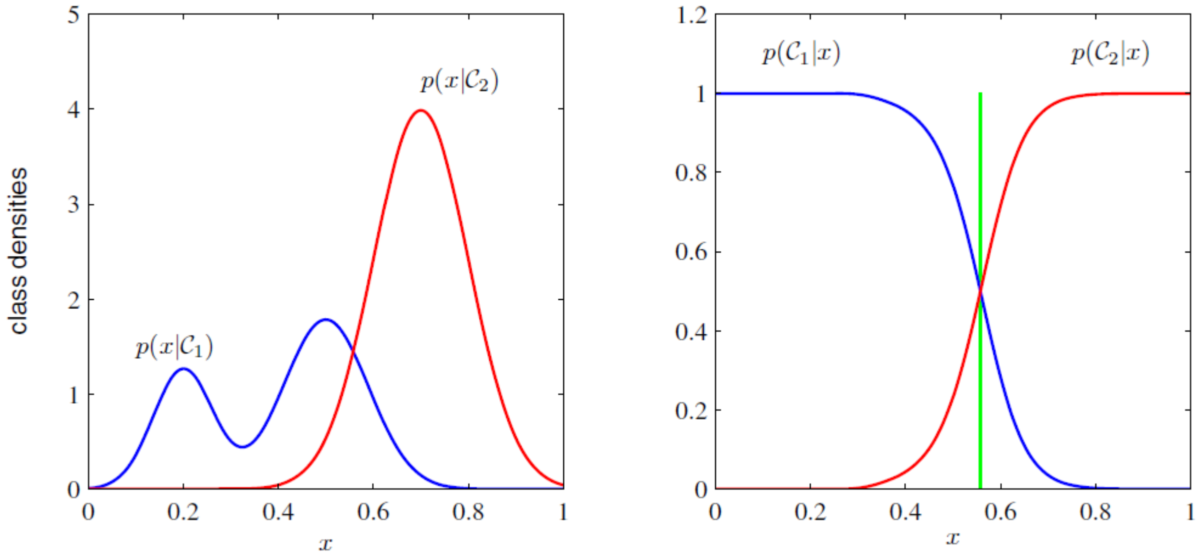
Soln : Bayesian Naïve Bayes Classifiers!

Discriminative vs Generative

- **Generative Models :** model the joint distribution p(x, Ck) directly and then normalize to obtain the posterior probabilities.

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

- Most demanding because it involves finding the joint distribution over both x and Ck. For many applications, x will have high dimensionality, and consequently we may need a large training set. if we only wish to make classification decisions, then it can be wasteful of computational resources but can be useful for detecting **outliers or novel classes**.



Discriminative vs Generative

- **Generative Models :** model the joint distribution p(x, Ck) directly and then normalize to obtain the posterior probabilities.

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

- **Easy to adapt to new data :** Use posterior probabilities as prior
- **Multi-Modal Data :** combining multiple modalities and domains

$$p(\mathbf{x}_{\mathrm{I}}, \mathbf{x}_{\mathrm{B}}|\mathcal{C}_k) = p(\mathbf{x}_{\mathrm{I}}|\mathcal{C}_k)p(\mathbf{x}_{\mathrm{B}}|\mathcal{C}_k).$$

- **Easy to fit?** very easy to fit generative classifiers. we can fit a naive Bayes model and an LDA model by simple counting and averaging. logistic regression requires solving a convex optimization problem which is much slower.
- **Fit classes separately?** In a generative classifier, we estimate the parameters of each class conditional density independently, so we do not have to retrain the model when we add more classes.
- **Well-calibrated probabilities?** Some generative models, such as naive Bayes, make strong independence assumptions which are often not valid
- Generative models can easily handle unlabelled data and missing features

Decision Theory

- Inference stage : Learning joint probability distribution $p(\mathbf{x}, \mathbf{t})$
- Decision stage : Specific prediction for the value of $\mathbf{t}$

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

- If our aim is to minimize the chance of assigning **x** to the wrong class, then we would choose the class having the higher posterior probability
- need a rule that assigns each value of **x** to one of the available classes,
- divide the input space into regions *Rk* called *decision regions* -> *decision boundaries* or *decision surfaces*.

$$\begin{aligned} p(\text{mistake}) &= p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1) \\ &= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\,\mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\,\mathrm{d}\mathbf{x}. \end{aligned}$$

Decision Theory

- Minimum misclassification rate decision rule, which assigns each value of *x* to the class having the higher posterior probability *p*(*Ck*/*x*).

$$\begin{aligned} p(\text{mistake}) &= p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1) \\ &= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\,\mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\,\mathrm{d}\mathbf{x}. \end{aligned}$$

$$\begin{aligned} p(\text{correct}) &= \sum_{k=1}^{K} p(\mathbf{x} \in \mathcal{R}_k, \mathcal{C}_k) \\ &= \sum_{k=1}^{K} \int_{\mathcal{R}_k} p(\mathbf{x}, \mathcal{C}_k)\,\mathrm{d}\mathbf{x} \end{aligned}$$

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