Linear and Quadratic Classifiers I — Generative models

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Generative Classifiers

We consider a (closed set) classification problem

We have a pattern $\boldsymbol{x}_t$ that we want to classify as belonging to one of k classes

Probabilistic model: we assume that $\boldsymbol{x}_t$ is a realization of R.V. $\boldsymbol{X}_t$

We also assume that its (unknown) class label can be described by R.V. $C_t \in \{1 \dots k\}$

$1 \dots k$ are the class labels[1]

[1] The actual values used to represent the classes are irrelevant, without loss of generality we assume classes are labeled using progressive integers. For binary problems, we will, in some cases, encode classes with $\{1, 0\}$.

Generative Classifiers

Optimal Bayes decision[2]: assign the class with highest posterior probability $c_t^* = \arg\max_c P(C_t = c|\boldsymbol{X}_t = \boldsymbol{x}_t)$

For example, we can consider an object classification task

$\boldsymbol{x}_t$ is the representation of an image

Labels represent what object is depicted (e.g. cat $= 1$, dog $= 2$, rabbit $= 3$, ...)

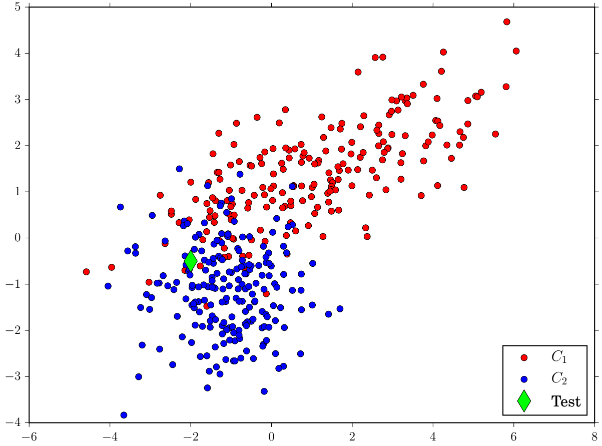
We want to find which label c_t is more likely for $\boldsymbol{x}_t$

For all labels $c \in \{1 \dots K\}$, we compute $P(C_t = c|\boldsymbol{X}_t = \boldsymbol{x}_t)$, i.e. the probability that the class C_t for the test sample t is c, conditioned on the observed value $\boldsymbol{X}_t = \boldsymbol{x}_t$

[2] Assuming uniform cost of errors

Generative Classifiers

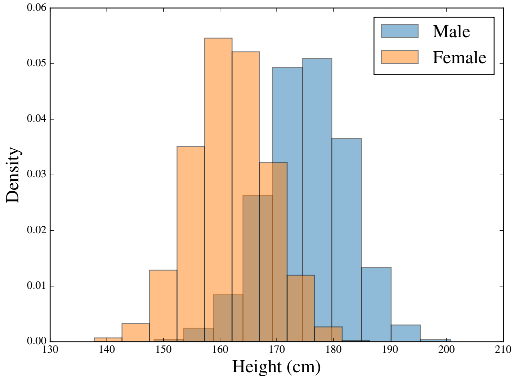
A binary example



What class is the green sample from?

Generative Classifiers

A univariate, binary example: forensics — infer the gender from the height



What's the gender of a 174 cm tall suspect?

Generative Classifiers

Simple model: assume that the samples are independent and distributed according to $\boldsymbol{X}_t, C_t \sim \boldsymbol{X}, C$, for any test sample t

Let the joint density of $\boldsymbol{X}, C$ be $f_{\boldsymbol{X},C}$

We can compute the joint likelihood for the hypothesized class c for the observed test sample $\boldsymbol{x}_t$:

$$f_{\boldsymbol{X}_t,C_t}(x_t, c) = f_{\boldsymbol{X},C}(x_t, c)$$

Since we are considering a closed-set classification problem, from Bayes rule we can compute the class posterior probability

$$P(C_t = c|\boldsymbol{X}_t = \boldsymbol{x}_t) = \frac{f_{\boldsymbol{X},C}(x_t, c)}{\sum_{c' \in \mathcal{C}} f_{\boldsymbol{X},C}(\boldsymbol{x}_t, c')}$$

Generative Classifiers

The joint density for $(\boldsymbol{X}_t, C_t)$ can be expressed as

$$f_{\boldsymbol{X}_t,C_t}(\boldsymbol{x}_t, c) = f_{\boldsymbol{X},C}(\boldsymbol{x}_t, c) = f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|c)P_C(c)$$

$P_C(c)$, or simply $P(c)$, is the prior probability for class c, and represents the probability of the class being c, before we observe the test sample (e.g. how likely we believe that a picture will depict a cat)

Usually, $P(c)$ is application-dependent: for example, in the desert we may have a prior probability for next day being rainy $P(rain) = 0.001$, whereas in the rain forest we may have $P(rain) = 0.5$

Our objective: modeling the class-conditional distribution $\boldsymbol{X}|C$, i.e. we want to estimate the density

$$f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|c)$$

Gaussian Classifier

We consider problems where the observations are continuous $\boldsymbol{x} \in \mathbb{R}$

How can we model $f_{X|C}(\boldsymbol{x}_t|c)$?

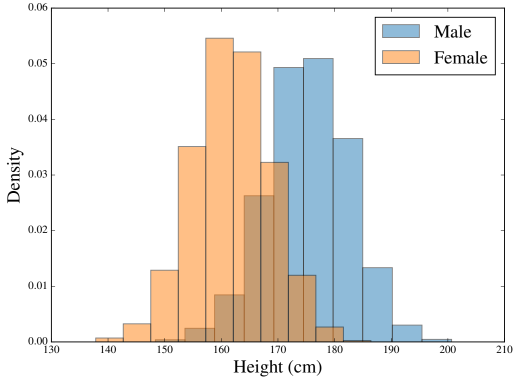
Of course, the answer depends on the data

In the following, we assume that the data of each class can be modeled by a (Multivariate) Gaussian Distribution

We will need to verify the performance of the model

Generative Classifiers

We start with a univariate example — gender inference

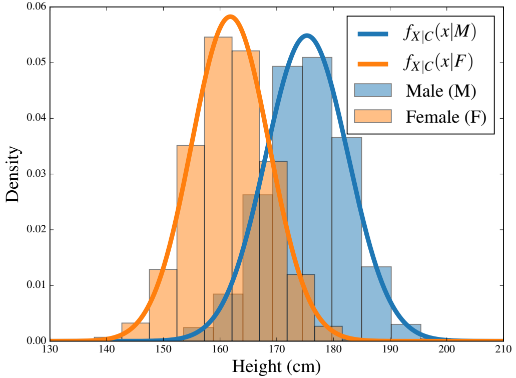


We assume we have a large set of height measurements for the population under consideration

Generative Classifiers

Intuitively, we can fit a Gaussian density over the samples of each class

We can use ML estimates to fit a Male ($C = M$) and a Female ($C = F$) Gaussian



Generative Classifiers

The ML parameters are the mean and variance of the samples of the Male and Female classes, respectively[3]

$$\mu_M = \frac{1}{N_M} \sum_{i|C_i=M} x_i \approx 175.33 \text{ cm} , \quad \sigma_M^2 = \frac{1}{N_M} \sum_{i|C_i=M} (x_i - \mu_M)^2 \approx 52.89 \text{ cm}^2$$

$$\mu_F = \frac{1}{N_F} \sum_{i|C_i=F} x_i \approx 161.82 \text{ cm} , \quad \sigma_F^2 = \frac{1}{N_F} \sum_{i|C_i=F} (x_i - \mu_F)^2 \approx 46.89 \text{ cm}^2$$

N_M and N_F are the number of male and female samples, and the sums extend over the male (first row) or female (second row) samples of the dataset

We are now able to compute the likelihood for the two classes for the 174 cm tall suspect

$$f_{X|C}(174|M) = \mathcal{N}(174|\mu_M, \sigma_M^2) \approx 0,05395$$
$$f_{X|C}(174|F) = \mathcal{N}(174|\mu_F, \sigma_F^2) \approx 0.01198$$

[3] In the following slides we will drop the unit of measurement

Generative Classifiers

It’s approximately 4.5 times more likely to observe a height of 174 cm in the male population

However, this is not sufficient to answer whether the sample is from a male or a female

We need to compute the class posterior probability, which depends also on the class prior probability

$$P(C = M|X = 174) = \frac{f_{X|C}(174|M)P(C = M)}{f_X(174)}$$
$$P(C = F|X = 174) = \frac{f_{X|C}(174|F)P(C = F)}{f_X(174)}$$

If we want to just compare the two probabilities, we don’t need to compute the normalization term $f_X(174)$

Gaussian Classifier

The class posterior ratio for the two hypotheses is

$$\frac{P(C=M|X=174)}{P(C=F|X=174)} = \frac{f_{X|C}(174|M)}{f_{X|C}(174|F)} \frac{P(C=M)}{P(C=F)}$$

The prior probabilities represent the probability that, a priori, we expect to observe a male or female sample

In this example, we may not have any knowledge of the suspect gender, so we may assume $P(C=M) = P(C=F) = \frac{1}{2}$

In this case

$$\frac{P(C=M|X=174)}{P(C=F|X=174)} = \frac{f_{X|C}(174|M)}{f_{X|C}(174|F)} \approx 4.5$$

i.e., the probability that the sample is from a male is 4.5 times higher than the probability that it is from a female

Gaussian Classifier

In other cases, we may have other information sources that lead us believe that the suspect is more likely to be from a specific gender.

As an example, we may believe for other reasons that the probability that the suspect is female is 90%: $P(C = F) = 0.9$ and $P(C = M) = 0.1$

In this case, the posterior ratio becomes

$$\frac{P(C = M|X = 174)}{P(C = F|X = 174)} = \frac{f_{X|C}(174|M)}{f_{X|C}(174|F)} \frac{P(C = M)}{P(C = F)} \approx \frac{4.5}{9} = \frac{1}{2}$$

i.e., the probability that the suspect is female is still twice the probability that the suspect is make, *even though* the evidence suggests otherwise

In this case, the evidence is not strong enough to change our prior belief.

Gaussian Classifier

We will now formalize the method we just employed in the example

We assume that our data, given the class, can be described by a Gaussian distribution

$$(\boldsymbol{X}_t | C_t = c) \sim (\boldsymbol{X} | C = c) \sim \mathcal{N}(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

We have one mean and one covariance matrix per class

If we knew $\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c$, then we could compute $f_{\boldsymbol{X}_t|C_t=c}$ as

$$f_{\boldsymbol{X}_t|C_t}(\boldsymbol{x}_t|c) = f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|c) = \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

We do not, however, know the values for the model parameters $\boldsymbol{\theta} = [(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \dots (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$

Gaussian Classifier

On the other hand, we have at our disposal a labeled training dataset

$$\mathcal{D} = \{(\boldsymbol{x}_1, c_1) \ldots (\boldsymbol{x}_n, c_n)\}$$

$\mathcal{X} = \{\boldsymbol{x}_1 \ldots \boldsymbol{x}_n\}$ are the observed samples

$\mathcal{C} = \{c_1 \ldots c_n\}$ are the corresponding class labels $c_i \in \{1 \ldots k\}$

We want to learn the model parameters from the data

Gaussian Classifier

We assume that, given the model parameters $\boldsymbol{\theta}$, observations are independent and identically distributed (i.i.d.)

$$[(\boldsymbol{X}_i, C_i) \perp\!\!\!\perp (\boldsymbol{X}_j, C_j)] \,|\boldsymbol{\theta}$$

and

$$\forall i, \quad (X_i, C_i)|\boldsymbol{\theta} \sim (X, C)|\boldsymbol{\theta}$$

i.e., we assume that both the training set and evaluation samples are independent (given the model parameters) and they are distributed in the same way

Gaussian Classifier

Since we assume Gaussian distribution for $X|C$, we have

$$(\boldsymbol{X}_i|C_i = c, \boldsymbol{\theta}) \sim (\boldsymbol{X}_t|C_t = c, \boldsymbol{\theta}) \sim (\boldsymbol{X}|C = c, \boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

i.e., the class-conditional distribution for all observations is a Gaussian with class-dependent mean $\boldsymbol{\mu}_c$ and class-dependent covariance matrix $\boldsymbol{\Sigma}_c$

Again, the model parameters are $\boldsymbol{\theta} = [(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \ldots (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$

We follow a frequentist approach, and we thus want to compute an estimator (or point estimate) $\boldsymbol{\theta}^*$ of the model parameters

We will then use the estimated parameters to compute

$$f_{\boldsymbol{X}_t|C_t}(\boldsymbol{x}_t|c) \approx \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_c^*, \boldsymbol{\Sigma}_c^*)$$

Gaussian Classifier

We have seen that a possible way to estimate the model parameters is to maximize the data (log-)likelihood

The likelihood for $\boldsymbol{\theta}$ is

$$\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}) &= f_{X_1 \dots X_n, C_1 \dots C_n|\boldsymbol{\theta}}(\boldsymbol{x}_1 \dots \boldsymbol{x}_n, c_1 \dots c_n|\boldsymbol{\theta}) \\
&= \prod_{i=1}^{n} f_{X,\boldsymbol{C}|\boldsymbol{\theta}}(\boldsymbol{x}_i, c_i|\boldsymbol{\theta}) \\
&= \prod_{i=1}^{n} f_{X|C,\boldsymbol{\theta}}(\boldsymbol{x}_i|c_i, \boldsymbol{\theta}) P(c_i) \\
&= \prod_{i=1}^{n} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{c_i}, \boldsymbol{\Sigma}_{c_i}\right) P(c_i)
\end{aligned}$$

where the factorization derives from the i.i.d. assumptions

Gaussian Classifier

We again consider the log-likelihood

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= \log \mathcal{L}(\boldsymbol{\theta}) \\ &= \sum_{i=1}^{n} \log \mathcal{N}\left(\boldsymbol{x}_i | \boldsymbol{\mu}_{c_i}, \boldsymbol{\Sigma}_{c_i}\right) + \sum_{i} \log P(c_i) \\ &= \sum_{c=1}^{k} \sum_{i|c_i=c} \log \mathcal{N}\left(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c\right) + \xi\end{aligned}$$

where ξ collects terms that do not depend on $\boldsymbol{\theta}$, and thus are irrelevant for the maximization with respect to $\boldsymbol{\theta}$.

The log-likelihood corresponds to a sum over all classes of the conditional log-likelihood of the samples belonging to each class

$$\ell(\boldsymbol{\theta}) = \sum_{c=1}^{k} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) + \xi \ , \quad \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) = \sum_{i|c_i=c} \log \mathcal{N}\left(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c\right)$$

Gaussian Classifier

We can thus maximize ℓ by separately maximizing the terms $\ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$

But $\ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$ is simply the log-likelihood of a Gaussian model for the data of class c

We are independently estimating the Gaussian densities that best describe the data of each class c

For univariate R.V.s, we have already shown that the ML solution corresponds to the class mean and variance

We now consider the general case for multivariate samples

Gaussian Classifier

The log-density for a Gaussian distribution $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is

$$\log \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{D}{2}\log 2\pi - \frac{1}{2}\log|\boldsymbol{\Sigma}| - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})$$

or, in terms of precision matrix $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$

$$\log \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{D}{2}\log 2\pi + \frac{1}{2}\log|\boldsymbol{\Lambda}| - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Lambda}(\boldsymbol{x}-\boldsymbol{\mu})$$

Gaussian Classifier

The log-likelihood $\ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$ can thus be expressed as

$$\ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) = k + \frac{N_c}{2} \log |\boldsymbol{\Lambda}_c| - \frac{1}{2} \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T \boldsymbol{\Lambda}_c (\boldsymbol{x}_i - \boldsymbol{\mu}_c)$$

We can rewrite the log-likelihood in different ways:

$$\ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) = k + \frac{N_c}{2} \log |\boldsymbol{\Lambda}_c| - \frac{1}{2} \operatorname{Tr}\left(\boldsymbol{\Lambda}_c \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c)(\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T\right) \tag{1}$$

$$\begin{aligned} &= k + \frac{N_c}{2} \log |\boldsymbol{\Lambda}_c| - \frac{1}{2} \sum_{i|c_i=c} \boldsymbol{x}_i^T \boldsymbol{\Lambda}_c \boldsymbol{x}_i + \boldsymbol{\mu}_c^T \boldsymbol{\Lambda}_c \sum_{i|c_i=c} \boldsymbol{x}_i - \frac{N_c}{2} \boldsymbol{\mu}_c^T \boldsymbol{\Lambda}_c \boldsymbol{\mu}_c \\ &= k + \frac{N_c}{2} \log |\boldsymbol{\Lambda}_c| - \frac{1}{2} \operatorname{Tr}\left(\boldsymbol{\Lambda}_c \sum_{i|c_i=c} \boldsymbol{x}_i \boldsymbol{x}_i^T\right) + \boldsymbol{\mu}_c^T \boldsymbol{\Lambda}_c \sum_{i|c_i=c} \boldsymbol{x}_i - \frac{N_c}{2} \boldsymbol{\mu}_c^T \boldsymbol{\Lambda}_c \boldsymbol{\mu}_c \end{aligned} \tag{2}$$

Gaussian Classifier

From (2) we observe that the log-likelihood depends on the data only through the statistics

$$\begin{aligned}Z_c &= N_c \\ \boldsymbol{F}_c &= \sum_{i|c_i=c} \boldsymbol{x}_i \\ \boldsymbol{S}_c &= \sum_{i|c_i=c} \boldsymbol{x}_i \boldsymbol{x}_i^T\end{aligned}$$

These are also called sufficient statistics: they collect all the information contained in the dataset that is relevant for the estimation of $\boldsymbol{\mu}_c$ and $\boldsymbol{\Sigma}_c$

Gaussian Classifier

We can find the maximum of ℓ_c by taking the derivatives of ℓ_c and setting them equal to 0:

$$\begin{cases} \nabla_{\boldsymbol{\Lambda}_c} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Lambda}_c) = \mathbf{0} \\ \nabla_{\boldsymbol{\mu}_c} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Lambda}_c) = \mathbf{0} \end{cases}$$

From (2), the derivative with respect to $\boldsymbol{\mu}_c$ is

$$\nabla_{\boldsymbol{\mu}_c} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Lambda}_c) = \boldsymbol{\Lambda}_c \sum_{i|c_i=c} \boldsymbol{x}_i - N_c \boldsymbol{\Lambda}_c \boldsymbol{\mu}_c$$

Solving for $\nabla_{\boldsymbol{\mu}_c} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Lambda}_c) = \mathbf{0}$ gives

$$\boldsymbol{\mu}_c = \frac{1}{N_c} \sum_{i|c_i=c} \boldsymbol{x}_i$$

i.e., the mean of samples belonging to class c

Gaussian Classifier

From (1), we can compute the derivative[4] w.r.t. $\boldsymbol{\Lambda}_c$:

$$\nabla_{\boldsymbol{\Lambda}_c} \ell_c(\boldsymbol{\mu}_c, \boldsymbol{\Lambda}_c) = \frac{N_c}{2} \boldsymbol{\Lambda}^{-T} - \frac{1}{2} \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^T$$

Assuming that $\sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^T$ is positive-definite (we can check that it's also symmetric), solving for $\boldsymbol{\Lambda}_c^{-1}$ gives

$$\boldsymbol{\Sigma}_c = \boldsymbol{\Lambda}_c^{-1} = \frac{1}{N_c} \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c)(\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T$$

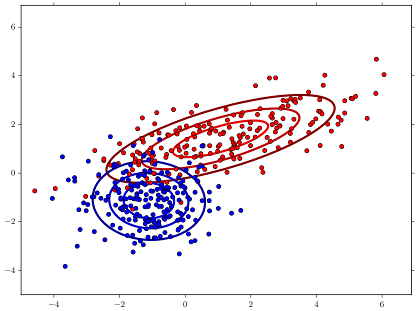
i.e., the covariance matrix of samples belonging to class c, computed using the data mean $\boldsymbol{\mu}_c$

[4]Since $\boldsymbol{\Lambda}_c$ is a precision matrix, it should be symmetric positive definite. We therefore should maximize ℓ_c under such constraint. In practice, we solve the problem for unconstrained $\boldsymbol{\Lambda}_c$, and then we check whether the unconstrained solution satisfies the constraints. Since it does, it's also the optimal solution for the constrained problem

Gaussian Classifier

Summarizing, the ML solution is given by

$$\boldsymbol{\mu}_c^* = \frac{1}{N_c} \sum_{i|c_i=c} \boldsymbol{x}_i \ , \quad \boldsymbol{\Sigma}_c^* = \frac{1}{N_c} \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c^*)(\boldsymbol{x}_i - \boldsymbol{\mu}_c^*)^T$$



We can then compute the likelihood of class c for test point $\boldsymbol{x}_t$ as

$$f_{\boldsymbol{X}_t|C_t}(\boldsymbol{x}_t|c) = f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|c) = \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_c^*, \boldsymbol{\Sigma}_c^*)$$

Gaussian Classifier

Let's now consider a binary task, with two classes[5] $C \in \{h_1, h_0\}$

We assign the label to a test sample $\boldsymbol{x}_t$ according to the highest posterior probability, comparing $P(C = h_1|\boldsymbol{x}_t)$ to $P(C = h_0|\boldsymbol{x}_t)$

We can express the comparison in terms of class posterior ratio

$$r(\boldsymbol{x}_t) = \frac{P(C = h_1|\boldsymbol{x}_t)}{P(C = h_0|\boldsymbol{x}_t)}$$

or, alternatively, in terms of its logarithm

$$\log r(\boldsymbol{x}_t) = \log \frac{P(C = h_1|\boldsymbol{x}_t)}{P(C = h_0|\boldsymbol{x}_t)}$$

[5]For binary problems it's common to label classes as 1 (target hypothesis, true hypothesis, ...) and 0 (non-target hypothesis, false hypothesis, null hypothesis, ...). As we have already said, the chosen labeling scheme is irrelevant for our discussion — we denote the class labels as h_1 and h_0

Gaussian Classifier

If the log-ratio is greater than 0, then the point will be assigned to class h_1, otherwise it will be assigned to class h_0

The class posterior ratio can be rewritten to make explicit its dependency on the likelihoods $f_{X|C}(\boldsymbol{x}_t|c)$ and prior class probabilities:

$$\begin{aligned}
\log r(\boldsymbol{x}_t) &= \log \frac{P(C = h_1|\boldsymbol{x}_t)}{P(C = h_0|\boldsymbol{x}_t)} \\
&= \log \frac{f_{X,C}(\boldsymbol{x}_t, h_1)}{f_X(\boldsymbol{x}_t)} \cdot \frac{f_X(\boldsymbol{x}_t)}{f_{X,C}(\boldsymbol{x}_t, h_0)} \\
&= \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)P(C = h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)P(C = h_0)} \\
&= \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)} + \log \frac{P(C = h_1)}{P(C = h_0)}
\end{aligned}$$

Gaussian Classifier

The first element of the sum is the log-likelihood ratio

$$llr(\boldsymbol{x}_t) = \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)}$$

It represents the ratio between the likelihood of observing the sample given that it belongs to h_1 or to h_0

The second term represents the prior (log)-odds. For a binary problem, we have

$$P(C = h_1) = \pi \ , \quad P(C = h_0) = 1 - P(C = h_1) = 1 - \pi$$

thus

$$\log r(\boldsymbol{x}_t) = \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)} + \log \frac{\pi}{1 - \pi}$$

Gaussian Classifier

As we have mentioned, π reflects the prior probability for class h_1 given a specific application

The first term, the log-likelihood ratio, is what our system should focus on providing — we want our system to be application-independent as much as possible

Whoever will use the system will plug the prior probabilities for his own task, and compute posterior log-probability ratios

Gaussian Classifier

The optimal decision is based on the comparison

$$\log r(\boldsymbol{x}_t) \gtrless 0$$

which means that we compare

$$\log r(\boldsymbol{x}_t) = \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)} + \log \frac{\pi}{1-\pi} \gtrless 0$$

i.e., we assign classes based on

$$llr(\boldsymbol{x}_t) = \log \frac{f_{X|C}(\boldsymbol{x}_t|h_1)}{f_{X|C}(\boldsymbol{x}_t|h_0)} \gtrless -\log \frac{\pi}{1-\pi}$$

Gaussian Classifier

The log-likelihood ratio acts as a score, with a probabilistic interpretation

Greater scores values imply our system favors class h_1, lower values mean it favors class h_0

The decision requires comparing the llr to a threshold t that depends on the application, through the class prior probability π

Later we shall see that we can (and should) also account for different costs for different kind of errors — we will show that this corresponds to using different effective priors

Gaussian Classifier

Let's see what kind of decision surfaces correspond to the llr of the Gaussian classifier with parameters $[(\boldsymbol{\mu}_1, \boldsymbol{\Lambda}_1^{-1}), (\boldsymbol{\mu}_0, \boldsymbol{\Lambda}_0^{-1})]$

We can compute the log–likelihood ratio

$$llr(\boldsymbol{x}) = \log \frac{\mathcal{N}(\boldsymbol{x}|h_1)}{\mathcal{N}(\boldsymbol{x}|h_0)} = \log \frac{\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_1, \boldsymbol{\Lambda}_1^{-1})}{\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_0, \boldsymbol{\Lambda}_0^{-1})}$$

The decision function is quadratic in $\boldsymbol{x}$:

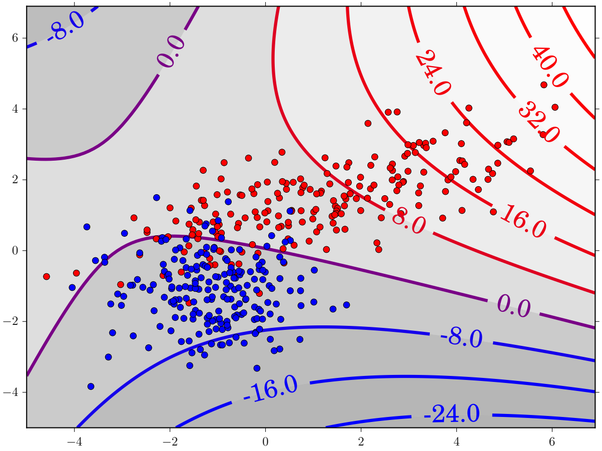
$$llr(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} + \boldsymbol{x}^T \boldsymbol{b} + c$$

with

$$\begin{aligned}
\boldsymbol{A} &= -\frac{1}{2}\left(\boldsymbol{\Lambda}_1 - \boldsymbol{\Lambda}_0\right) \\
\boldsymbol{b} &= \left(\boldsymbol{\Lambda}_1 \boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_0 \boldsymbol{\mu}_0\right) \\
c &= -\frac{1}{2}\left(\boldsymbol{\mu}_1^T \boldsymbol{\Lambda}_1 \boldsymbol{\mu}_1 - \boldsymbol{\mu}_0^T \boldsymbol{\Lambda}_0 \boldsymbol{\mu}_0\right) + \frac{1}{2}\left(\log|\boldsymbol{\Lambda}_1| - \log|\boldsymbol{\Lambda}_0|\right)
\end{aligned}$$

Gaussian Classifier

Binary problem — decision boundaries



Gaussian Classifier

For multiclass problems $C \in \{h_1, h_2 \ldots h_k\}$ we can compute closed-set posterior probabilities as

$$P(C = h_i | \boldsymbol{x}_t) = \frac{f_{\boldsymbol{X}|C}(\boldsymbol{x}_t | h_i) P(h_i)}{\sum_{h' \in \{h_1, h_2 \ldots h_k\}} f_{\boldsymbol{X}|C}(\boldsymbol{x}_t | h') P(h')}$$

Optimal decisions require choosing the class with highest posterior probability $c_t^* = \arg\max_h P(C = h | \boldsymbol{x}_t)$. Posterior probabilities are proportional to

$$P(C = h_i | \boldsymbol{x}_t) \propto f_{\boldsymbol{X}|C}(\boldsymbol{x}_t | h_i) P(h_i)$$

and the proportionality factor is the same for all classes

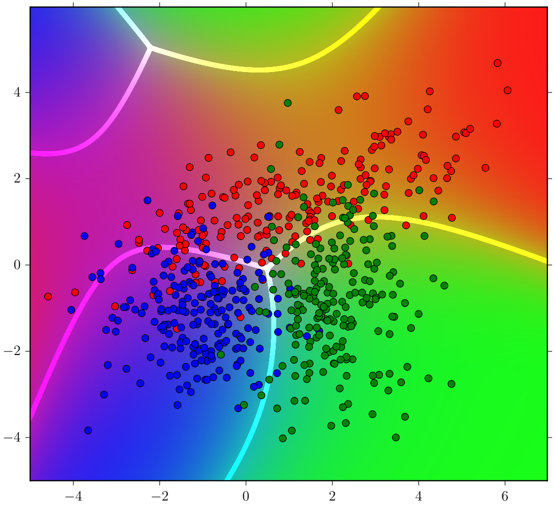
Optimal decisions can thus be computed as

$$c_t^* = \arg\max_h f_{\boldsymbol{X}|C}(\boldsymbol{x}_t | h) P(h) = \arg\max_h \log f_{\boldsymbol{X}|C}(\boldsymbol{x}_t | h) + \log P(h)$$

Again, the first term should be the output of the classifier, whereas the second term $\log P(h)$ depends on the application

Gaussian Classifier

3 class problem — class posteriors and pair-wise boundaries



Gaussian Classifier

The Gaussian model requires computing a mean and a covariance matrix for each class

If the samples are few compared to their dimensionality, then the estimates can be inaccurate

The issue is more evident for covariance matrices, since they have $\frac{D\times(D+1)}{2}$ independent elements

The off-diagonal terms of $\boldsymbol{\Sigma}_c$ represent the covariances of the different components of our feature vectors

Gaussian Classifier

If we know that, for each class, the different components are approximately independent, we can simplify the estimate assuming that the the distribution of $X|C$ can be factorized over its components

$$f_{\boldsymbol{X}|C}(\boldsymbol{x}|c) \approx \prod_{j=1}^{D} f_{X_{[j]}|C}(x_{[j]}|c)$$

where $x_{[j]}$ is the j-th component of $\boldsymbol{x}$ (not to be confused with $\boldsymbol{x}_j$, the j-th dataset sample)

This model is called Naive Bayes

The assumption is not tied to any specific distribution — we can even employ different distributions for different components

Gaussian Classifier

The naive Bayes assumption, combined with Gaussian assumptions, models the distributions $f_{X_{[j]}|C}(x_{[j]}|c)$ as univariate Gaussians

$$f_{X_{[j]}|C}(x_{[j]}|c) = \mathcal{N}(x_{[j]}|\mu_{c,[j]}, \sigma^2_{c,[j]})$$

We can again compute the ML estimates. The log-likelihood factorizes over sample components:

$$\mathcal{L}(\boldsymbol{\theta}) \propto \prod_{i=1}^{n} \prod_{j=1}^{D} \mathcal{N}\left(\boldsymbol{x}_{i,[j]}|\mu_{c_i,[j]}, \sigma^2_{c_i,[j]}\right)$$

$$\ell(\boldsymbol{\theta}) = \xi + \sum_{c=1}^{k} \sum_{i|c_i=c} \sum_{j=1}^{D} \log \mathcal{N}\left(\boldsymbol{x}_{i,[j]}|\mu_{c,[j]}, \sigma^2_{c,[j]}\right)$$

$$= \xi + \sum_{j=1}^{D} \sum_{c=1}^{k} \sum_{i|c_i=c} \log \mathcal{N}\left(\boldsymbol{x}_{i,[j]}|\mu_{c,[j]}, \sigma^2_{c,[j]}\right)$$

Gaussian Classifier

We can optimize the log-likelihood independently for each component

For each component, we have the log-likelihood of a Gaussian model

The ML solution is

$$\mu^*_{c,[j]} = \frac{1}{N_c} \sum_{i|c_i=c} x_{i,[j]} \ , \quad \sigma^2_{c,[j]} = \frac{1}{N_c} \sum_{i|c_i=c} (x_{i,[j]} - \mu_{c,[j]})^2$$

Gaussian Classifier

We can observe that the density for a sample $\boldsymbol{x}$ can be expressed as

$$f_{X|C}(\boldsymbol{x}|c) = \prod_{j=1}^{D} \mathcal{N}(x_{[j]}|\mu^*_{c,[j]}\sigma^2_{c,[j]}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

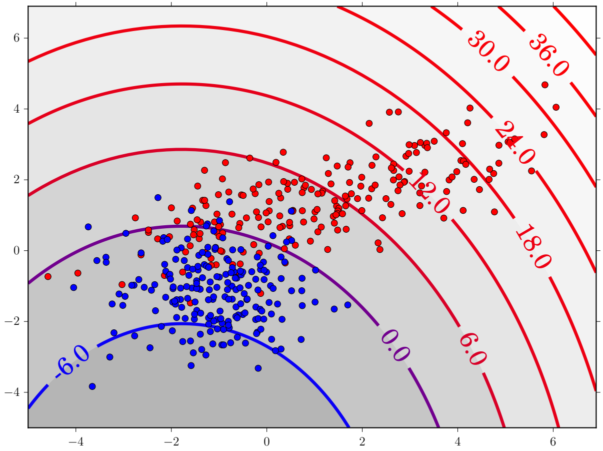
where

$$\boldsymbol{\mu}_c = \begin{bmatrix} \mu_{c,[1]} \\ \mu_{c,[2]} \\ \vdots \\ \mu_{c,[D]} \end{bmatrix} , \quad \boldsymbol{\Sigma}_c = \begin{bmatrix} \sigma^2_{c,[1]} & 0 & \dots & 0 \\ 0 & \sigma^2_{c,[2]} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma^2_{c,[D]} \end{bmatrix}$$

The naive Bayes Gaussian classifier corresponds to a Multivariate Gaussian classifier with diagonal covariance matrices (this does not hold for a generic density!)

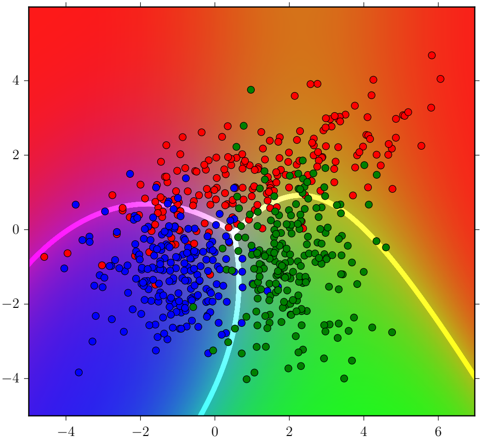
Gaussian Classifier

Binary problem — naive Bayes Gaussian classifier



Gaussian Classifier

3 class problem — naive Bayes Gaussian classifier



Gaussian Classifier

Another common Gaussian model assumes that the covariance matrices of the different classes are tied

- Class-independent noise: $\boldsymbol{x}_{c,i} = \boldsymbol{\mu}_c + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Lambda}^{-1})$
- Badly-conditioned problems (large dimensional data, small number of samples) — A single shared covariance matrix can be more easily estimated

The tied covariance model assumes that

$$f_{X|C}(\boldsymbol{x}|c) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma})$$

i.e., each class has its own mean $\boldsymbol{\mu}_c$, but the covariance matrix is the same for all classes

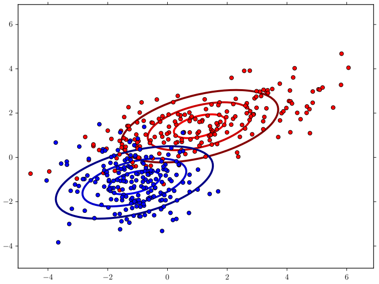
Gaussian Classifier

Again, we can estimate the parameters using the ML framework. In this case the log-likelihood does not factorize over classes

The ML solution is

$$\boldsymbol{\mu}_c^* = \frac{1}{N_c} \sum_{i|c_i=c} \boldsymbol{x}_i \ , \quad \boldsymbol{\Sigma}^* = \frac{1}{N} \sum_c \sum_{i|c_i=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c)(\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T$$

where N is the number of samples $N = \sum_{c=1}^{k} N_c$



Gaussian Classifier

Let’s compute the binary log–likelihood ratios for the tied model:

$$\begin{aligned} llr(\boldsymbol{x}) &= \log \frac{f_{X|C}(\boldsymbol{x}|h_1)}{f_{X|C}(\boldsymbol{x}|h_0)} \\ &= \log \frac{\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_1, \boldsymbol{\Lambda}^{-1})}{\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_0, \boldsymbol{\Lambda}^{-1})} \\ &= \boldsymbol{x}^T \boldsymbol{b} + c \end{aligned}$$

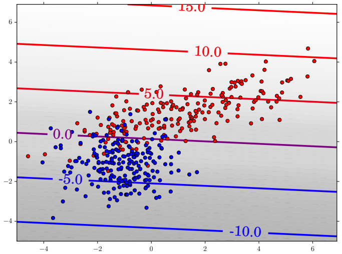
with

$$\begin{aligned} \boldsymbol{b} &= \boldsymbol{\Lambda}\left(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0\right) \\ c &= -\frac{1}{2}\left(\boldsymbol{\mu}_1^T \boldsymbol{\Lambda} \boldsymbol{\mu}_1 - \boldsymbol{\mu}_0^T \boldsymbol{\Lambda} \boldsymbol{\mu}_0\right) \end{aligned}$$

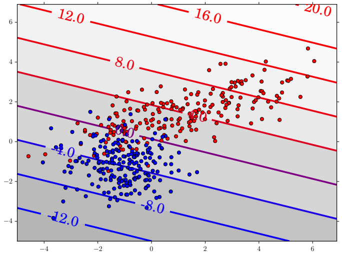
i.e., a linear function of $\boldsymbol{x}$

Gaussian Classifier

Binary classifier — tied covariances



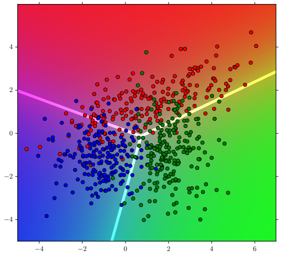
Multivariate



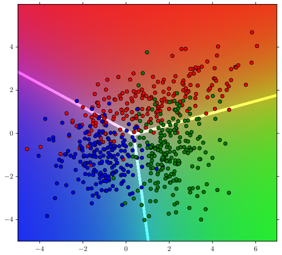
Naive Bayes

Gaussian Classifier

Multiclass classifier — tied covariances



Multivariate



Naive Bayes

Gaussian Classifier

The model is also closely related to LDA

Remember that two–class LDA looks for the direction which maximizes the generalized Rayleigh quotient

$$\frac{\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}}$$

with

$$\begin{aligned}\boldsymbol{S}_W &= \boldsymbol{\Lambda}^{-1} \\ \boldsymbol{S}_B &= (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T\end{aligned}$$

We have seen that we can solve the problem by applying the following transformations

$$\begin{aligned}\boldsymbol{x}' &= \boldsymbol{\Lambda}^{\frac{1}{2}} \boldsymbol{x} \\ \boldsymbol{S}'_W &= \boldsymbol{I} \\ \boldsymbol{S}'_B = \boldsymbol{\Lambda}^{\frac{1}{2}} &(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \boldsymbol{\Lambda}^{\frac{1}{2}}\end{aligned}$$

Gaussian Classifier

Since $\boldsymbol{v} = \boldsymbol{\Lambda}^{\frac{1}{2}}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$ is a vector, the leading eigenvector of $\boldsymbol{S}_B'$ is

$$\boldsymbol{\nu} = \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|}$$

Projection over the LDA subspace is, up to a scaling factor, given by

$$\boldsymbol{w}^T \boldsymbol{x} = k \cdot \boldsymbol{x}^T \boldsymbol{\Lambda} \left(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0\right)$$

This corresponds to the classification rule of the Gaussian model with tied covariances!

Indeed, LDA assumes that all classes have the same within–class covariance

The Gaussian model with one covariance per class is also known as Quadratic Discriminant Analysis

Gaussian Classifier

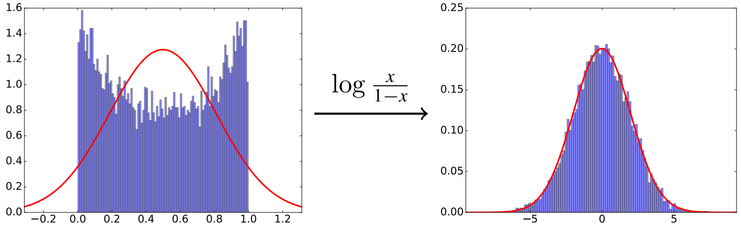
Practical considerations:

- If data is high-dimensional, PCA can simplify the estimation
- PCA also allows removing dimensions with very small variance (e.g. in the MNIST dataset, pixels that are white for all images regardless of the digit)
- Multivariate models perform better if we have enough data to reliably estimate the covariance matrices
- Naive Bayes can simplify the estimation, but may perform poorly if data are highly correlated
- Tied covariance models can capture correlations, but may perform poorly when classes have very different distributions — on the other hand, if we have reason to believe that covariances should be very similar, then the model will provide a more reliable estimate

Gaussian Classifier

Practical considerations:

- If a Gaussian model is not adequate for our data we can use different distributions that are more appropriate
- Alternatively, the Gaussian model may still be effective for transformed data



Multiclass Gaussian Classifier

MNIST — Error rates for Gaussian classifier

Classifier	PCA (100)	PCA (50)	PCA (9)	PCA + LDA (100 $\rightarrow$ 9)
Naive Tied Gaussian	13.7%	14.4%	25.0%	$\boxed{12.3\%}$
Tied Gaussian	$\boxed{12.3\%}$	12.6%	23.7%	$\boxed{12.3\%}$
Naive Gaussian	12.2%	12.3%	23.4%	11.4%
Gaussian	4.3%	$\boxed{3.6\%}$	12.2%	10.2%

Multiclass Gaussian Classifier

Comments:

- The best model is the unconstrained MVG — classes have significantly different within class covariance matrices
- The Naive Bayes assumption is not good in this case (strong within-class correlations)
- PCA helps reducing the complexity — from 100 to 50 dimensions we have a significant gain. If we reduce too much we have bad results again

Multiclass Gaussian Classifier

Comments:

- Tied model + LDA achieve the same performance as Tied model without LDA — The LDA subspace contains all the information used by the tied model
- The Naive tied model, without LDA, performs slightly worse — it ignores within-class correlations.
- Our implementation of LDA whitens the within-class covariance matrix — Tied naive model and Tied model are equivalent, since $\boldsymbol{\Sigma} = \boldsymbol{I}$

Modeling discrete values

We now consider a problem characterized by discrete features

For the moment, we assume we have a single categorical feature $x \in \{1 \dots m\}$.

For example, we may want to predict a cat gender from the fur color

Modeling discrete values

The categorical feature is the fur color, for example

$$x \in \{white, black, orange, gray, bi\text{-}color, calico, ...\}$$

Also in this case, we have a set of labeled training samples

$$\mathcal{D} = \{(x_1, c_1) \dots (x_n, c_n)\}$$

Each sample x_i is simply the fur color of the i-th cat sample, and c_i is the gender label

Modeling discrete values

We also assume that samples are i.i.d. (as in the Gaussian case)

We want to compute the probabilities

$$P(X_t = x_t | C_t = c) = \pi_{c,x_t}$$

for the different hypotheses c, for the observed test sample x_t

In our example, these are the probabilities of observing fur color x_t under the different gender hypotheses $c \in \{female, male\}$ (e.g. $P(X_t = white | C_t = female)$)

$\boldsymbol{\pi}_c = (\pi_{c,1} \dots \pi_{c,m})$ are the model parameters for class c, with

$$\sum_{i=1}^{m} \pi_{c,i} = 1$$

Modeling discrete values

Again, we can adopt a frequentist approach and estimate the ML solution for $\boldsymbol{\Pi} = (\boldsymbol{\pi}_1 \dots \boldsymbol{\pi}_k)$ (k is again the number of classes)

We can express the likelihood for the training set as

$$\mathcal{L}(\boldsymbol{\Pi}) = \prod_{i=1}^{n} P(X_i = x_i | C_i = c_i) P(C_i = c_i)$$

where $c_i \in \{1 \dots k\}$ is the class of the i-th sample

Modeling discrete values

For example, if our dataset consists of[6]

(black, male), (orange, male), (black, female), (orange, male),
(white, male), (white, female), (white, male), (white, female),
(black, female), (calico, female)

the likelihood is simply the product

$$\begin{aligned}\mathcal{L}(\mathbf{\Pi}) = & P(X_1 = black|C_1 = male)P(C_1 = male)\times \\ & P(X_2 = orange|C_2 = male)P(C_2 = male)\times \\ & P(X_3 = black|C_3 = female)P(C_3 = female)\times \\ & \vdots \\ & P(X_{10} = calico|C_{10} = female)P(C_{10} = female)\end{aligned}$$

[6] We assume we have associated each color to an integerer value $\{1 \ldots m\}$, and that the gender labels are associated to $\{0, 1\}$

Modeling discrete values

The log-likelihood is given by

$$
\begin{aligned}
\ell(\mathbf{\Pi}) &= \sum_{i=1}^{n} \log P(X_i = x_i | C_i = c_i) + \xi \\
&= \sum_{i=1}^{n} \log \pi_{c_i, x_i} + \xi \\
&= \sum_{c=1}^{k} \sum_{i | c_i = c} \log \pi_{c, x_i} + \xi \\
&= \sum_{c=1}^{k} \ell_c(\boldsymbol{\pi}_c) + \xi
\end{aligned}
$$

where

$$
\ell_c(\boldsymbol{\pi}_c) = \sum_{i | c_i = c} \log \pi_{c, x_i}
$$

Again, the log-likelihood can be expressed as a sum of terms, each depending on a separate subset of the parameters (those of class c)

Modeling discrete values

We can thus estimate the parameters by independently optimizing $\ell_c(\boldsymbol{\pi}_c)$

We have

$$\begin{aligned}\ell_c(\boldsymbol{\pi}_c) &= \sum_{i|c_i=c} \log \pi_{c,x_i} \\ &= \sum_{j=1}^{m} N_{c,j} \log \pi_{c,j}\end{aligned}$$

where $N_{c,j}$ is the number of times we observed $x_i = j$ in the dataset for class c (i.e. the number of times the features of class c were equal to j)

In our example we would have

$$\begin{array}{llll} N_{female,black} = 2 & N_{female,orange} = 0 & N_{female,white} = 2 & N_{female,calico} = 1 \\ N_{male,black} = 1 & N_{male,orange} = 2 & N_{male,white} = 2 & N_{male,calico} = 0 \end{array}$$

Modeling discrete values

Solving for π_{c,x_i} is a bit more complex than in the Gaussian case, since we have the constraint that $\sum_{j=1}^{m} \pi_{c,j} = 1$

In the following we drop subscript c, thus we look for the maximizer of

$$f(\boldsymbol{\pi}) = \sum_{j=1}^{m} N_j \log \pi_j$$

subject to

$$\sum_{j=1}^{m} \pi_j = 1$$

A solution can be obtained by means of Lagrange multipliers

We look for stationary points of

$$L(\boldsymbol{\pi}) = f(\boldsymbol{\pi}) - \lambda \left(\sum_{j=1}^{m} \pi_j - 1 \right) = \sum_{j=1}^{m} N_j \log \pi_j - \lambda \left(\sum_{j=1}^{m} \pi_j - 1 \right)$$

Modeling discrete values

We need to solve

$$\begin{cases} \frac{\partial L}{\partial \pi_i} = 0 \,, & \forall i = 1 \dots m \\ \frac{\partial L}{\partial \lambda} = 0 \end{cases}$$

We have

$$\frac{\partial L}{\partial \pi_i} = \frac{N_i}{\pi_i} - \lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = 1 - \sum_{j=1}^{m} \pi_j = 0$$

We can verify that $\lambda \neq 0$, so that

$$\pi_i = \frac{N_i}{\lambda}$$

Modeling discrete values

From the derivative with respect to λ we thus have

$$\sum_{j=1}^{m} \pi_j = \sum_{j=1}^{m} \frac{N_j}{\lambda} = \frac{1}{\lambda} \sum_{j=1}^{m} N_j = 1$$

thus

$$\lambda = \sum_{j=1}^{m} N_j = N$$

where $N = \sum_{j=1}^{m} N_j$ is the number of samples for the considered class

We finally have

$$\pi_i = \frac{N_i}{N}$$

i.e., the frequency with which we observed value i in the class

Modeling discrete values

The ML solution for each class is thus

$$\pi^*_{c,i} = \frac{N_{c,i}}{N_c}$$

We can compute the predictive distribution for x_t as

$$P(X_t = x_t | C_t = c) = \pi^*_{c,x_t}$$

In our example, we would have

$$N_{male} = 5 \quad N_{female} = 5$$

thus

$$\pi^*_{female,black} = 0.4 \quad \pi^*_{female,orange} = 0 \quad \pi^*_{female,white} = 0.4 \quad \pi^*_{female,calico} = 0.2$$
$$\pi^*_{male,black} = 0.2 \quad \pi^*_{male,orange} = 0.4 \quad \pi^*_{male,white} = 0.4 \quad \pi^*_{male,calico} = 0$$

Modeling discrete values

If we have more than one categorical attribute, we may model their joint probability as a categorical R.V. with values given by all possible combinations of the attributes

In practice, the number of elements would quickly become intractable

We can adopt again a naive Bayes approximation and assume that features are independent

We can obtain ML estimates for each feature, and then combine them:

$$P(\boldsymbol{X}_t = \boldsymbol{x}_t | C_t = c) = \prod_j \pi^j_{c, x_{t,[j]}}$$

where j denotes the feature index

Modeling discrete values

We now consider an extended version of the problem, where features represent occurrences of events

Typical examples are topic or language modeling

We may, for example, represent a text in terms of the words that appear inside

Different topics will result in different sequences of words

Modeling all possible combinations of words is impractical, since the number of categories would grow exponentially with the number of words

Modeling discrete values

As an approximation, we may represent documents in terms of occurrences of single words

Note that such model ignores the order in which words appear — we may improve the model by considering pairs or triplets of words

Thus, we have feature vectors $\boldsymbol{x} = (x_{[1]} \dots x_{[m]})$, where each $x_{[i]}$ represents the number of times we observed word i in the document

Modeling discrete values

We have seen that occurrences can be modeled by multinomial distributions

Thus, for each class c, we have a set of parameters

$$\boldsymbol{\pi}_c = (\pi_{c,1} \dots \pi_{c,m})$$

that represents the probability of observing a single instance of word i

The probability for feature vector $\boldsymbol{x}$ is given by the multinomial density

$$P(\boldsymbol{X} = \boldsymbol{x} | C = c) = \frac{\left(\sum_{j=1}^{m} x_{[j]}\right)!}{\prod_{j=1}^{m} x_{[j]}!} \prod_{j=1}^{m} \pi_{c,j}^{x_{[j]}} \propto \prod_{j=1}^{m} \pi_{c,j}^{x_{[j]}}$$

Modeling discrete values

Again, we can write the likelihood of the model — as in the previous case, the likelihood factorizes over classes, thus

$$\ell(\boldsymbol{\Pi}) = \sum_c \ell_c(\boldsymbol{\pi}_c) + \xi$$

with

$$\ell_c(\boldsymbol{\pi}_c) = \sum_{i|c_i=c} \sum_{j=1}^{m} x_{i,[j]} \log \pi_{c,j}$$

Note that we did not write the multinomial coefficient since it's constant with respect to $\boldsymbol{\Pi}$, and thus can be absorbed in ξ.

Modeling discrete values

Also in this case we can express the log-likelihood as

$$\ell_c(\boldsymbol{\pi}_c) = \sum_{j=1}^{m} N_{c,j} \log \pi_{c,j}$$

where $N_{c,j}$ is the total number of occurrences of event j (word j) in the samples of class c:

$$N_{c,j} = \sum_{i|c_i=c} x_{i,[j]}$$

To solve the problem, we notice that it has exactly the same form as the one we solved for the categorical case

Modeling discrete values

Thus, the ML solution is again

$$\pi_{c,j} = \frac{N_{c,j}}{N_c}$$

where, in this case, N_c is the total number of words for class c

$$N_c = \sum_j N_{c,j} = \sum_{i|c_i=c} \sum_{j=1}^{m} x_{i,[j]}$$

$\pi_{c,j}$ is therefore again the relative frequency of word j in class c

Modeling discrete values

Again, we write the log-likelihood ratio for a two class problem (we use the expression of the multinomial log-probability — notice that the binomial coefficient can be simplified and thus disappears from the final expression):

$$\begin{aligned} llr(\boldsymbol{x}) &= \log \frac{P(\boldsymbol{X} = \boldsymbol{x} | C = h_1)}{P(\boldsymbol{X} = \boldsymbol{x} | C = h_0)} \\ &= \sum_{j=1}^{m} x_{[j]} \log \pi_{h_1,j} - \sum_{j=1}^{m} x_{[j]} \log \pi_{h_0,j} \\ &= \boldsymbol{x}^T \boldsymbol{b} \end{aligned}$$

with

$$\boldsymbol{b} = (\log \pi_{h_1,1} - \log \pi_{h_0,1}, \ldots \log \pi_{h_1,m} - \log \pi_{h_0,m})$$

Again, we have linear decision functions

Modeling discrete values

An example: inferring programming language

We consider the problem of automatically inferring whether a file is written in C or Python

We consider a simple model based on the occurrences of punctuation characters: `{} [] () : ; . ,`

We treat open and closed brackets of the same kind as a single symbol

We model scripts in terms of occurrences of the aforementioned symbols

Modeling discrete values

Let's consider the following training set

	{}	[]	()	:	;	.	,
C script 1	6	8	14	1	10	1	7
C script 2	8	10	14	0	11	1	7
C script 3	12	22	34	1	21	2	13
C script 4	4	6	10	1	6	1	4
C total	30	46	72	3	48	5	31
Py script 1	6	14	30	6	2	16	16
Py script 2	2	8	14	3	1	9	8
Py script 3	4	14	26	7	2	15	14
Py total	12	36	70	16	5	40	38

Modeling discrete values

The ML estimate for the model parameters are the symbol frequencies for each class :

	{}	[ ]	( )	:	;	.	,
π_C	0.128	0.196	0.306	0.013	0.204	0.021	0.132
π_{Py}	0.055	0.166	0.323	0.074	0.023	0.184	0.175

To infer the class of an unknown script, we need to compute class posterior.

In this case, the task is binary so we compute log-likelihood ratios $llr(\boldsymbol{x})$, where $\boldsymbol{x}$ is the vector of occurrences of the symbols in the test script

The log-likelihood ratio can be expressed as $llr(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{b}$

Modeling discrete values

Each element of $\boldsymbol{b}$ is $b_i = \log \frac{\boldsymbol{\pi}_{C,[i]}}{\boldsymbol{\pi}_{Py,[i]}}$

	`{}`	`[]`	`()`	`:`	`;`	`.`	`,`
$\boldsymbol{b} \approx$	0.837,	0.165,	-0.052,	-1.754,	2.182,	-2.159,	-0.283

The model parameters already tell us what symbols are most discriminant

Observing `;` is much more likely for C scripts

Observing `:` or `.` is much more likely for Python scripts

Round brackets are not very discriminant

Modeling discrete values

We consider two test scripts:

	{}	[ ]	( )	:	;	.	,
Test script $\boldsymbol{x}_1$ (C)	2	10	12	0	1	1	0
Test script $\boldsymbol{x}_2$ (Py)	2	18	16	3	0	1	1

The llr for the first script is $llr(\boldsymbol{x}_1) \approx 2.7$, i.e. it's more likely that we observe the occurrences of $\boldsymbol{x}$ in C scripts

For the second script we have $llr(\boldsymbol{x}_2) \approx -3.9$, i.e. it's significantly more likely that we observe the occurrences in $\boldsymbol{x}_2$ in Python scripts

Class posteriors can be computed once we choose class priors

With uniform priors, $\boldsymbol{x}_1$ would be assigned to C class, and $\boldsymbol{x}_2$ to Python class

Modeling discrete values

Practical considerations:

- Rare words can cause problems: if a word does not appear in a topic we will estimate a probability $\pi_{c,j} = 0$. Any test sample that contains the word will have 0 probability of being from class c
- We can mitigate the issue introducing pseudo-counts, i.e. assuming that each topic contains a sample were all words appear a (fixed) number of times
- In practice, we can add a fixed values to the class occurrences N_c before computing the ML solution
- This corresponds to a Maximum-a-posterior estimate using a Dirichlet prior distribution (we won't see the details in this course)

Modeling discrete values

Practical considerations:

- Bayesian treatment of the hyperparameters is a more appropriate way to deal with limited sample sizes (but we will not analyze Bayesian models)
- We can consider pairs of words, triplets of words and so on if we want to partially account for correlations
- We can also combine different models (categorical, multinomial, Gaussian, ...) through a naive Bayes assumption

Modeling discrete values

Some additional comments on the discrete models for categorical events:

- We can model a dataset of categorical samples as n independent categorical R.V.s $X_i \in \{1 \dots m\}$.
- Each variable represents a token.
- The distribution is described by a vector of probabilities $\boldsymbol{\pi}$ that allow computing $P(X = j) = \pi_j$

Modeling discrete values

Some additional comments on the discrete models for categorical events:

- Alternatively, we can model the dataset in terms of occurrences of events.
- We have a random vector $\boldsymbol{Y} = (Y_1 \dots Y_m)$ whose components are R.V. Y_i corresponding to the number of occurrences of event i in the dataset.
- Again, the distribution is described by a vector of probabilities $\boldsymbol{\pi}$ that represent probabilities of single events

The two models are related by

$$Y_j = \sum_{i=1}^{n} \mathbb{I}\left[X_i = j\right]$$

Modeling discrete values

As we have seen, in both cases the ML solution for $\boldsymbol{\pi}$ corresponds to the relative frequencies of occurrences. Indeed, we can go further and show that the two models are equivalent

Considering only samples of a single class, in the first case the log-likelihood for a given class is given by

$$\ell_X(\boldsymbol{\pi}) = \sum_{i=1}^{n} \log \pi_{x_i} = \sum_{j=1}^{m} N_j \log \pi_j$$

whereas in the second case

$$\ell_Y(\boldsymbol{\pi}) = \log \frac{\left(\sum_{j=1}^m y_{[j]}\right)!}{\prod_{i=1}^m y_{[j]}!} + \sum_{j=1}^{m} y_j \log \pi_j = \xi + \sum_{j=1}^{m} N_j \log \pi_j$$

Modeling discrete values

The corresponding likelihoods $\mathcal{L}_X(\boldsymbol{\pi})$ and $\mathcal{L}_Y(\boldsymbol{\pi})$ are proportional:

$$\mathcal{L}_X(\boldsymbol{\pi}) \propto \mathcal{L}_Y(\boldsymbol{\pi})$$

Therefore:

- Maximum likelihood estimates will be the same
- Bayesian posterior probabilities for model parameters will be the same (again, we will not go into details of Bayesian models)
- Inference will be the same

Modeling discrete values

The first point is straightforward

Regarding the last point, we can observe that, for a given test sample, the class conditional likelihoods are also proportional

$$f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|c) = \zeta(\boldsymbol{y}_t) \cdot f_{\boldsymbol{Y}|C}(\boldsymbol{y}_t|c)$$

Thus, binary log-likelihood ratios are equal

$$\log \frac{f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|h_1)}{f_{\boldsymbol{X}|C}(\boldsymbol{x}_t|h_0)} = \log \frac{f_{\boldsymbol{Y}|C}(\boldsymbol{y}_t|h_1)}{f_{\boldsymbol{Y}|C}(\boldsymbol{y}_t|h_0)}$$

and similarly for class posteriors:

$$P(C_t = c|\boldsymbol{X} = \boldsymbol{x}) = \frac{f_{X|C}(\boldsymbol{x}_t|c)P(c)}{\sum_{c'} f_{X|C}(\boldsymbol{x}_t|c')P(c')} = \frac{f_{Y|C}(\boldsymbol{y}_t|c)P(c)}{\sum_{c'} f_{Y|C}(\boldsymbol{y}_t|c')P(c')} = P(C_t = c|\boldsymbol{Y} = \boldsymbol{y})$$